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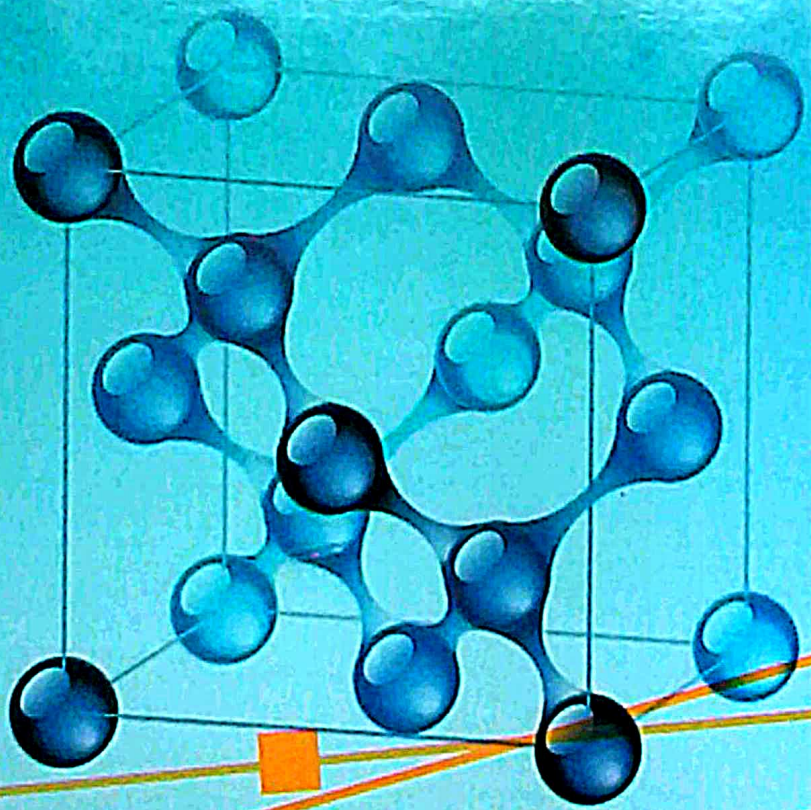
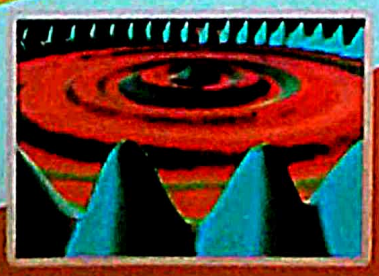
SOLID STATE PHYSICS

K.K. Sharma B.S. Satyal





KALYANI

As per CBCS Syllabus

SOLID STATE PHYSICS

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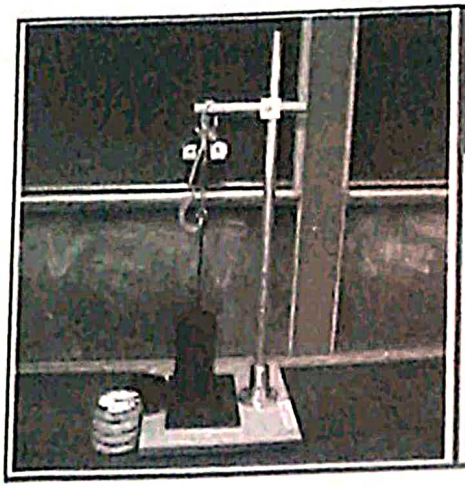
UNIT – I

1. *CRYSTAL STRUCTURE*

2. *ELEMENTARY LATTICE DYNAMICS*



Chapter 1

CRYSTAL STRUCTURE

1.1 INTRODUCTION

There are in general four states or phases of matter, *viz.*, solid, liquid, gas and plasma. Some other states like Bose-Einstein condensates, neutron degenerate matter and quark-gluon plasma also occur in extreme low temperature, extreme density and very high energy colour charged matter situations. The first four states are low energy states or classical states whereas degenerate matter, Bose-Einstein condensates, super conductivity, photonic matter and Fermionic condensate are high-energy states or modern states of matter. Quark-gluon plasma is very high energy state in which elementary particles, quarks become free and able to move independently in a sea of subatomic particles called gluons.

Solids have a definite shape and fixed volume. Liquids have no definite shape but fixed volume. Gases do not have definite shape and volume but are compressible fluids which conform to the shape of its container and even possess a tendency to expand to fill the container.

Plasmas have free charged particles usually in equal numbers. Usually plasmas respond strongly to electromagnetic forces. The study of physics that deals with solids is known as *solid state physics*. Basically, solid state physics is main branch of condensed matter physics which deals with solids as well as liquids.

Many scientists have contributed immensely to know what was special about the interior of solids. Nicolaus Steno (1638-1686), a dutch scientist was the first to study in 1669 that whatever was the shape and size of the crystals, the angle between the corresponding faces was the same. He used quartz crystals and this work was carried further by Leeuwenhoek (1632-1723) a dutch scientist in 1695, Domenico Gugleilimini (1655-1710) in 1688 published the same with other crystals. The observations of Nicolaus Steno were confirmed by Rome Delisle (1736-1790) in 1772. Abbe Hauy (1743-1822), a French Scientist in 1784 studied in detail the fundamental building block of the crystals. He cut off calcite crystals in different directons and concluded that the smallest building block is a rhombohedral piece which is independent of the crystal from which it was obtained. This smallest building block was termed as a unit cell.

Point to Remember

Hauy laid the foundation for the science of crystallography and is known as "Father of Crystallography".

Thus the science of determining the arrangements of atoms in the structure of the crystal came to be known as **Crystallography.** This word is made of crystal and graph. The crystal in Greek means cold drop or frozen drop. The word "Graph" in Greek means "I write". Prior to 1910, the crystallography was a subject of interest mainly to geologists and mineralogists. After 1910, the discovery of diffraction of X-rays by crystals led to the development of a powerful method for the exploration of the internal arrangements of atoms in the crystals.

Hence we shall study the physics of solids dealing with the study of crystals and of electrons in crystals using Bragg's law in this chapter. The crystallography is a branch of physics which deals with the study of all possible types of crystals and the physical properties of crystalline solids by the determination of their actual structure by using X-rays, neutron beams and electron beams.

1.2 SOLIDS : AMORPHOUS AND CRYSTALLINE MATERIALS

All solids have the property of incompressibility, rigidity and mechanical strength. Many atoms come closer together to form solid. The elementary particles in the atoms interact with each other resulting in a change in the behaviour. This behaviour of solid may be quite different from the behaviour of individual atom. The nature of atoms, their internal structures and the inter atomic forces and manner of arrangements of atoms determine the formation of a solid.

The solids have been classified into two categories on the basis of X-ray diffraction studies

(i) Crystalline solids

(ii) Amorphous solids

Crystalline Solids : When the constituent atoms of a solid are arranged in a definite, regular and repeated geometric pattern throughout the entire three dimensional network of the crystal, then the solid is called a crystalline solid.

Rock salt, quartz, mica, sugar, calcite, alum, ice, methanol, copper sulphate, sulphur and diamond are some examples of crystalline solids. The properties of crystalline solids are

(i) In crystalline solids, the constituent atoms, ions or the molecules are arranged in a definite regular geometric pattern.

(ii) Crystalline solids possess definite geometric shape.

(iii) The potential energy of the configuration of the constituent particles is minimum in the crystalline solids *i.e.* they are found in stable state.

(iv) There is a long range order in the structure of the crystalline solids.

(v) Periodicity in the arrangement of atoms, ions or molecules extends over many million atomic diameters.

(vi) Crystalline solids have sharp melting points *i.e.* they suddenly convert into liquid state at a definite temperature.

(vii) Crystalline solids are anisotropic *i.e.* their physical properties like electrical conductivity, thermal conductivity, thermal expansion, refractive index, mechanical strength etc. are different in different directions.

(viii) Crystalline solids are generally bounded by flat surfaces.

(ix) Crystalline solids are practically incompressible.

(x) Crystalline solids are considered as true solids.

(xi) Crystalline solids give a clean surface after cleaving them with a knife rather than an irregular breakage.

Point to Remember

Crystalline solids are those substances whose constituent particles possess a regular orderly arrangement.

Classification of Crystalline Solids : Various categories of the crystalline solids are classified depending upon the type of constituent particles and the nature of intermolecular forces between them. Broadly, the crystalline solids are divided into four categories.

(i) Ionic solid

(ii) Molecular solid

(iii) Covalent or Network solid

(iv) Metallic solid

Ionic solids are solids consisting of oppositely charged ions. They are composed of positively charged cations and negatively charged anions. These ions are held together by electrostatic forces. In the case of sodium chloride (NaCl) ionic solid is composed of simple ions whereas in the case of ammonium nitrate (NH_4NO_3), ionic solid is composed of polyatomic ions with NH_4^+ and NO_3^- ions. Some characteristics of ionic solids are

- they possess high melting point and boiling point due to strong electrostatic force of attraction.
- they are usually soluble in a polar solvent but not in a non polar solvent.
- they are basically insulators of electricity as the ions are not free to move. But they become good conductors in an aqueous solution as the ions become free.
- they are hard and brittle because their stability depends upon the preservation of their geometric pattern.

Molecular solids are solids consisting of molecules. They are further divided into three types depending upon the nature of the molecules.

(i) Non-polar molecular solids contain non-polar molecules like H_2, Cl_2, etc. or noble gas molecules. Weak vanderWaal's force or dispersion force is the attractive force between them and due to this, these molecules have low melting and boiling points. These molecules are soft in nature and are insulators of electricity.

(ii) Polar molecular solids contain polar molecules like HCl, SO_2 etc. Strong dipole-dipole force of attraction between these molecules is responsible for these solids to be soft, non-conductors of electricity. These solids exist in gaseous or liquid form at room temperature and pressure with melting and boiling points higher than non-polar molecules.

(iii) Hydrogen bonded molecular solids contain particles which are bonded with hydrogen bond like water, NH_3, HF etc. Due to strong hydrogen bond these molecules have a high melting and boiling points. They exist as volatile liquid or soft solids at room temperature and pressure.

Covalent or Network solids are the solids consisting of atoms of the same or different elements connected to each other by covalent bond. Here a network of covalent bonds is formed throughout the crystal and they form a giant molecule. Diamond, graphite and silicon carbide (SiC) etc. are some examples of covalent solids. These solids are hard, brittle and have high melting and boiling points. Covalent solids are insulators with the exception of graphite as graphite has a free fourth electron in its outer shell.

Metallic solids are the solids consisting of metal atoms. The attractive force between the positively charged metal ion and mobile valence electron is known as metallic bond which holds the metal ions together. Due to the strong metallic bonds, metals can maintain a regular structure and have high melting and boiling points. These solids possess high electrical and thermal conductivity. Mellalic solids are malleable and ductile. They have bright lustre and colour due to free electrons.

Point to Remember
Metal is a sea of mobile electrons.

Amorphous Solids : When the constituent atoms of a solid are not arranged in a definite geometrical pattern but are arranged in a random manner, then the solid is called an amorphous solid.

Glass, cement, polymers, rubber talc powder and many plastics are some examples of amorphous solids.

Point to Remember
The Greek word amorphous means without any form. The amorphous solids are also called glassy solids

The properties of amorphous solids are :

(i) Amorphous solids do not possess definite geometrical shape.

(ii) Amorphous solids are not bounded by flat surfaces.

(iii) Amorphous solids do not have equally strong bonds.

(iv) There may be short range order in the structure of amorphous solids *i.e.* the particles are arranged in a regular manner upto a small region only.

(v) Amorphous solids do not have sharp melting point *i.e.* these solids first soften and then finally melt.

(vi) Amorphous solids are isotropic in nature *i.e.* their physical properties remain in all directions.

(vii) Amorphous solids are considered as super cooled liquids of high viscosity.

(viii) Amorphous solids are not considered as true solids. Due to short range order, small parts of amorphous solids may be crystalline and rest may be non-crystalline. So they are known as **pseudo solids.**

(ix) Unlike crystalline solid, amorphous solids do not give a clean surface after cleavage with a knife. Rather, they undergo an irregular breakage.

(x) Amorphous solids do not exhibit rigidity. Deformation could be done by bending or compressing these solids.

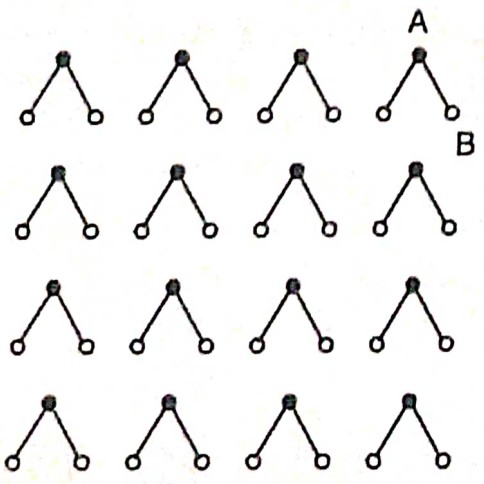
The scientific study of the amorphous solids began in the twentieth century inspite of long history of practical usage of the ordinary glass. Amorphous solids are prepared by various procedures other than the traditional liquid cooling. Amorphous semiconductor used for solar cells is one example. The methods generally applied to prepare the amorphous solids by physical and chemical procedures are as follows :

(i) rapid cooling of liquid.
(ii) mechanical milling of crystal. Here milling signifies the moving of particles constituting the solid in a large group in a haphazard irregular direction.
(iii) deposition of vapour onto a cold substrate.
(iv) compression or a depression of crystal.
(v) bombardment of particle onto a crystal.
(vi) gelation i.e. to freeze a liquid. The gelation is a process of formation of a gel from a solution.
(vii) precipitation by chemical reaction.
(viii) dehydration of hydrate crystals.

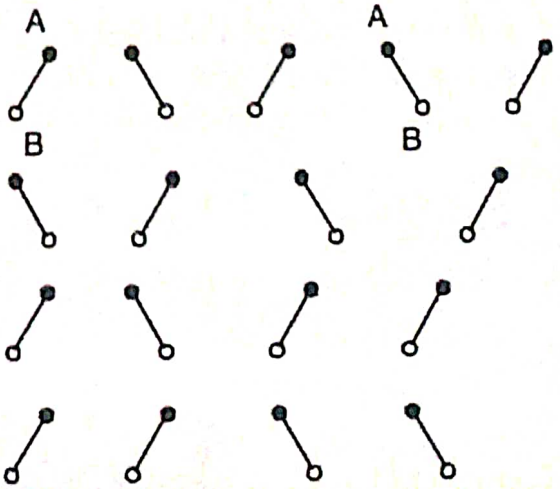
Structural Difference between Crystalline Solids and Amorphous Solids : The basic difference between the crystalline solids and amorphous solids is that crystalline solids possess long range order whereas the amorphous solids have a short range order. Fig. 1.1 (a) represents the placement of particles A and B represented by big filled circle and small empty circle respectively in a solid. Here one atom of type A is surrounded by two atoms of type B such that a group of one atom of type A and two atoms of type B repeats itself in a regular periodic fashion to show the structure of crystalline solids. Fig. 1.1 (b) represents the placement of particles A and B such that there is no regular periodic arrangement of atoms to show the structure of amorphous solids. For the sake of simplicity, only a two dimensional arrangement of atoms has been shown in Fig. 1.1.

Point to Remember

Unlike liquids, in which the atoms are free to move within the volume of the liquid in amorphous solids the atoms are rigidly fixed.



(a)



(b)

Fig. 1.1

1.6

1.3 LATTICE TRANSLATION VECTORS

A true solid is composed of regular and periodic arrangements of particles, *viz.* atoms, molecules or ions, extended over the large volume of crystal. The study of arrangement of particles in a crystal will become simple if we replace the repeating unit by a point. Then we can describe the crystal as a geometrical arrangement of points in a space. To understand the concept of arrangement of particles, we consider a two dimensional crystal structure as shown in Fig. 1.2. Here, a group of two atoms are taken as a unit represented by an open circle (O) and a filled circle (•) which repeats itself regularly. The crystal as a whole may be divided into two parts–the crystal lattice and the basis.

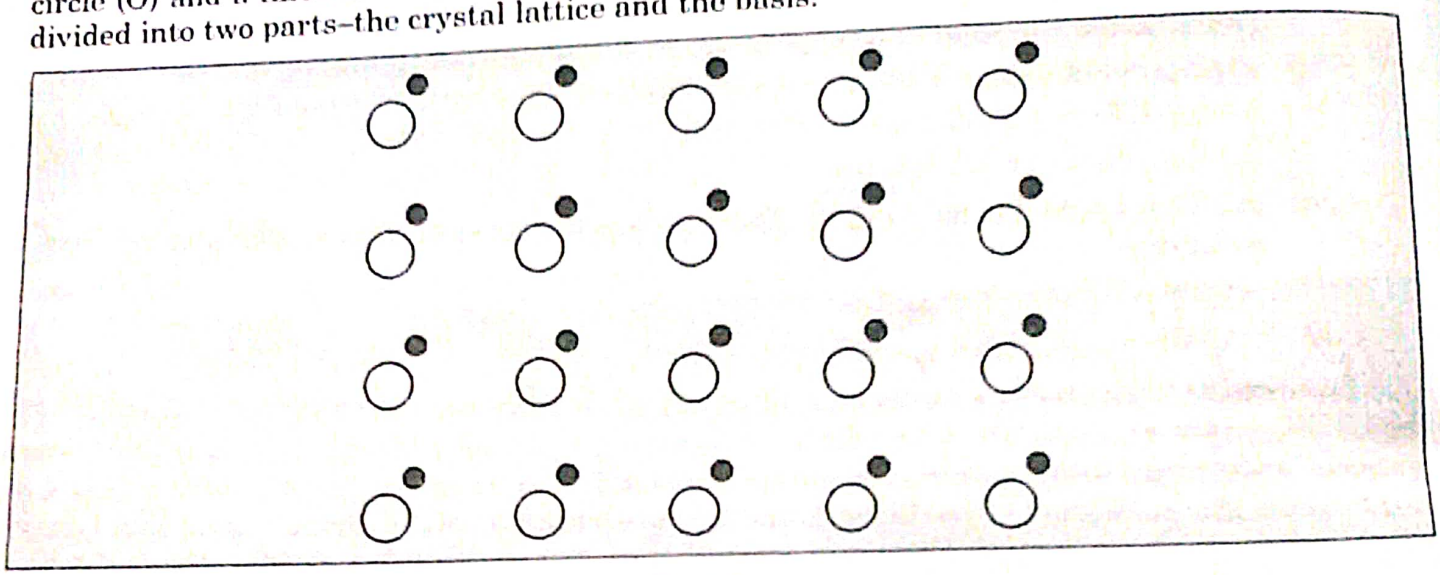


Fig. 1.2.

Crystal lattice : A crystal lattice is a regular, infinite, periodic arrangement of geometrical points in the space in such a way that the total energy of configuration is minimum so as to obtain the actual crystal structure.

Infact the crystal lattice is an array of points in space in which each point has the same surroundings. Each point on the crystal lattice is called a lattice point or a lattice site.

Basis : Basis is the set of particles–atoms, molecules or ions placed on each lattice point to give rise to a crystal. Thus, the logical relation for a crystal is

Lattice + Basis = Crystal structure

The crystal structure is obtained by joining each atom or group of atoms to lattice points. Due to the regularity of the structure, the environment about all the lattice points is identical. We can take any lattice point O as origin as shown in Fig. 1.3.

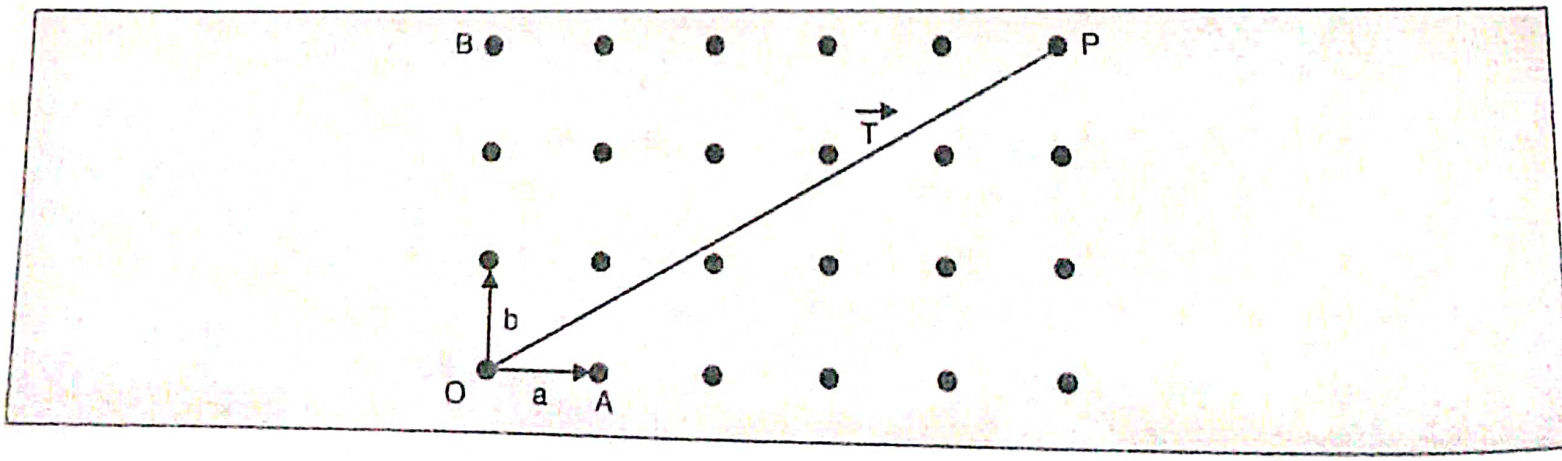


Fig. 1.3

Point to Remember

Translationally periodic arrangement of points in space is called a lattice.

The lattice points along OA are at equal distances a and along OB are at equal distances b. Thus, any lattice point P can be described in terms of a vector $\bar{T}$ as

$$T = n_1 \vec{a} + n_2 \vec{b}$$

where n_1 and n_2 are integers and T is known as the **translation vector** or crystal translation operator. In Fig. 1.3, $n_1 = 5$ and $n_2 = 3$

So that the given translation vector $\bar{T}$ is represented as

$$T = 5\vec{a} + 3\vec{b}$$

Actually, the crystal lattice is three dimensional so the arrangement of atoms in three dimensional lattice is identical to one for two dimensional crystal lattice. Any lattice point in three dimensional space is given by

$$\bar{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$$

where lengths $\vec{a}$, $\vec{b}$ and $\vec{c}$ are known as lattice parameters or lattice vectors. The directions of lattice vectors are called as crystalline axes or lattice axes. Different directions are assigned for the lattice axes. So the selection of translation vector is not unique.

1.4 UNIT CELL

The atoms are arranged in a regular and orderly manner in crystalline solids. Hence, it is convenient to express the structure of a crystal by taking only a small group of atoms to show the arrangement of atoms in the crystal. Imagine this small group of atoms located in a cell. Such a cell is called a unit cell. The lattice points can be split up into a number of unit cells. This can be obtained by joining the points by a regular network of lines as shown in Fig. 1.4.

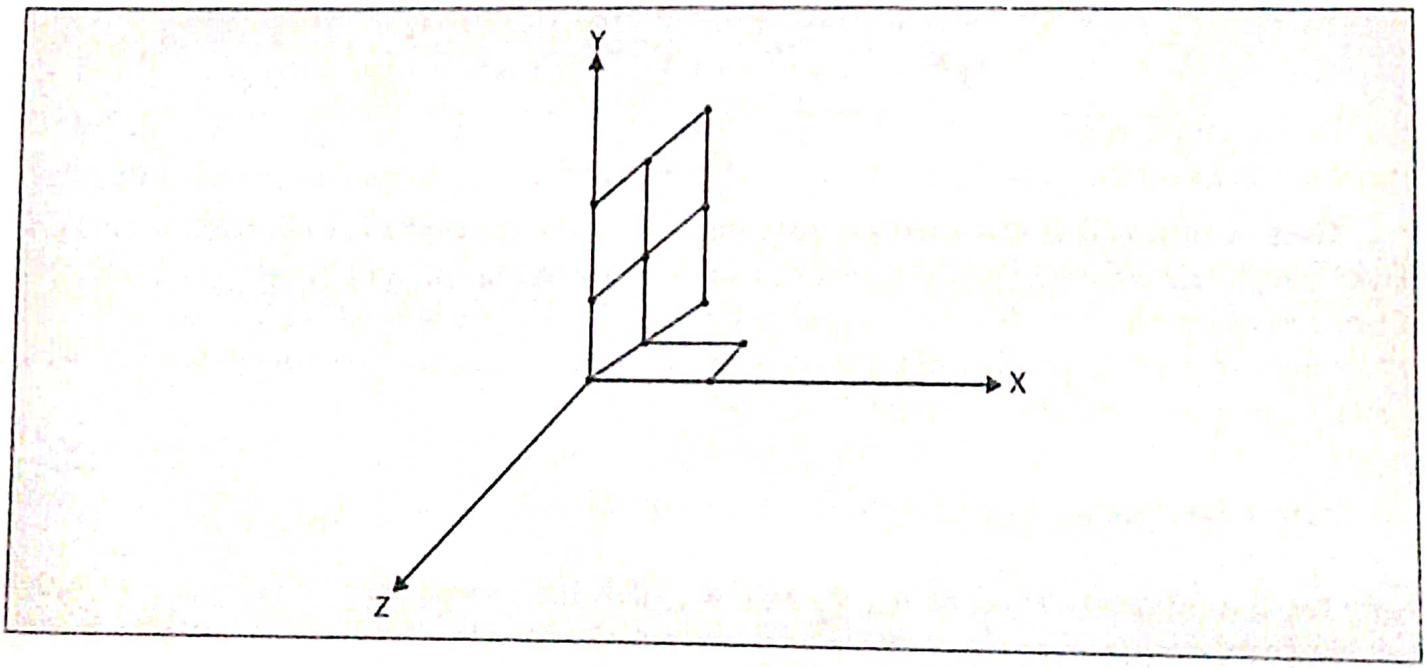


Fig. 1.4

A unit cell is the smallest repeating unit in space lattice which when repeated over and over again results in a crystal of the given substance.

The entire crystal can easily be described by the description of a unit cell. So a unit cell is a building block which makes the whole crystal and it represents all the characteristics of the crystal.

Point to Remember

For the study of the crystal, we can deal with the study of unit cell rather than the whole crystal.

Following parameters fully describe a unit cell :

(i) Lattice parameters a, b and c *i.e.* the distances which give lengths of the edges of the unit cell.

(ii) Interfacial angles α, β and γ which give angles between the three imaginary axes OX, OY and OZ.

Fig. 1.5 shows the lattice parameters and interfacial angles. The lattice angle α is the angle between $\vec{b}$ and $\vec{c}$, β is the angle between $\vec{c}$ and $\vec{a}$ and γ is the angle between $\vec{a}$ and $\vec{b}$.

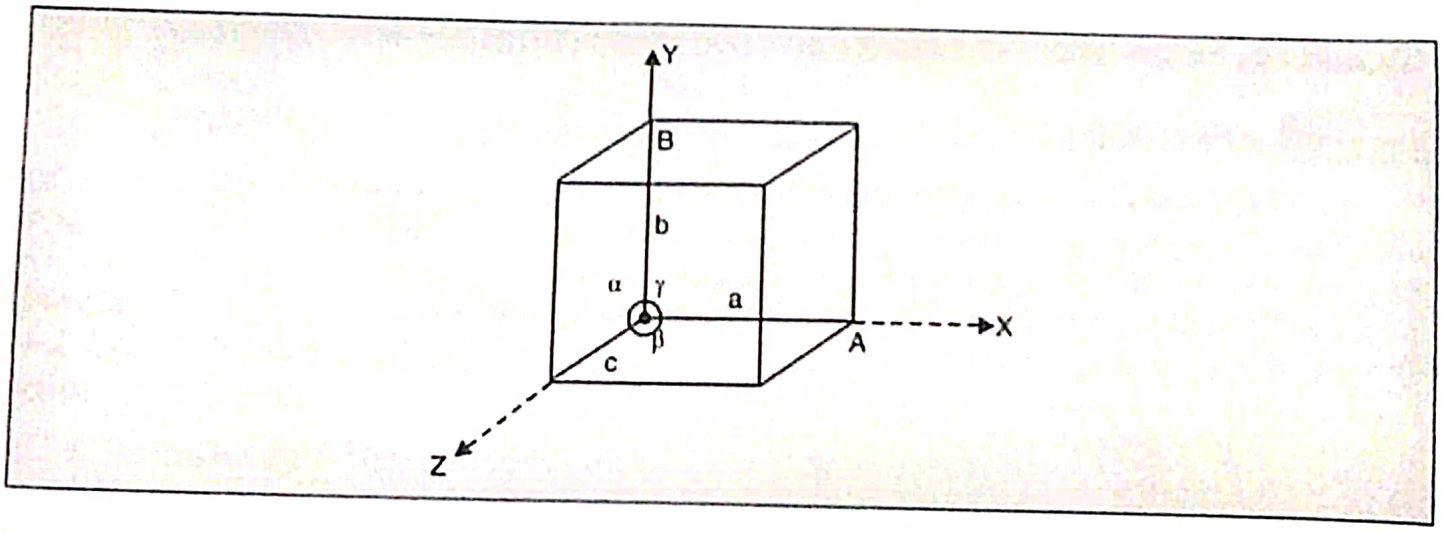


Fig. 1.5

Thus, a unit cell is the smallest pattern unit of the arrangement of atoms in a crystal from which the whole crystal can be built up by translating the unit parallel to itself in the direction of its edges by distances equal to the lengths of the edges. Though a unit cell can be chosen in an infinite number of ways, it is certainly preferable to choose in such a unit which exibits the symmetry of the crystal.

Primitive translational vector : If the equation, $T = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$ is satisfied only for the integral values of n_1, n_2 and n_3, then the translational vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$ are called primitive translational vectors. For a given lattice the choice of the primitive translational vectors is not unique.

Point to Remember

The intercepts OA along the X-axis, OB along Y-axis and OC along Z axis in the unit cell shown in Fig 1.5 are known as primitives and are represented as $\vec{a}$, $\vec{b}$ and $\vec{c}$.

Primitive Cell : The primitive cell is the smallest unit cell in volume constructed by primitives. Here, the lattice points are only at the corner of a unit cell. In two dimensions the cell (i) and cell (iii) are the primitive cells as shown in Fig. 1.6. If a unit cell consists of more than one atom, then it is not a primitive cell. A primitive cell is a unit cell that contains exactly one lattice point. The unit cell (ii) and unit cell (iv) in Fig. 1.6 are non-primitive unit cells.

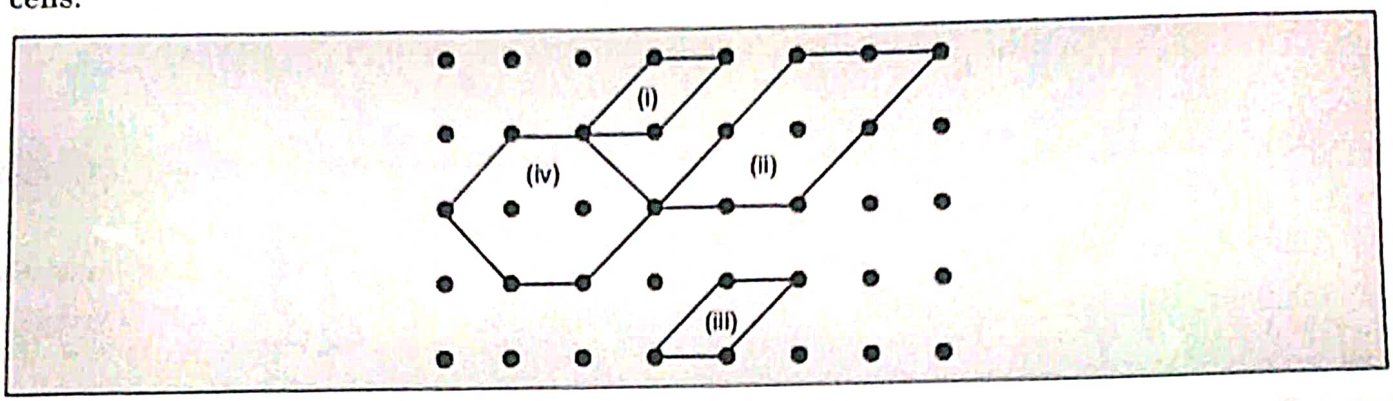


Fig. 1.6.

A two dimensional primitive cell is a parallelogram which may have orthogonal angles or equal lengths or both as shown in Fig. 1.7.

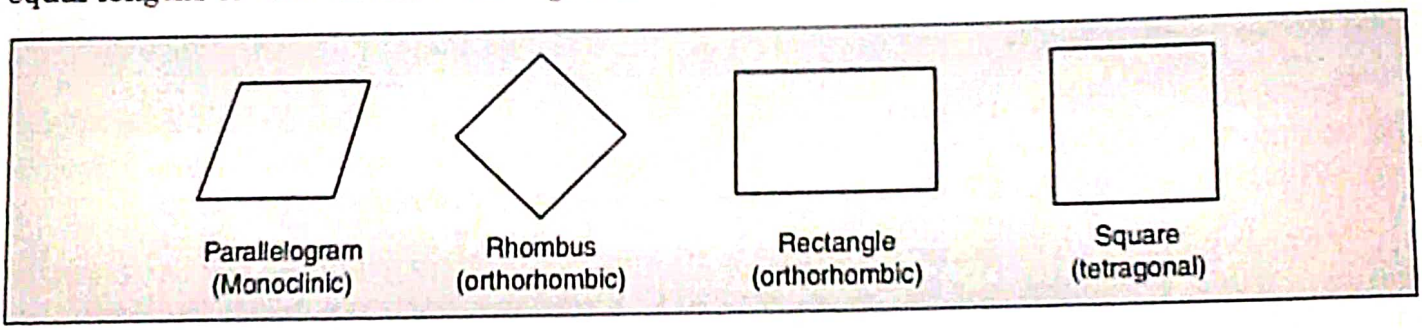


Fig. 1.7.

If we look closely, the total part of the lattice points from each corner which contributes in forming the primitive unit cell is one. The total contributing lattice points in one unit cell formation in Fig. 1.8 is one.

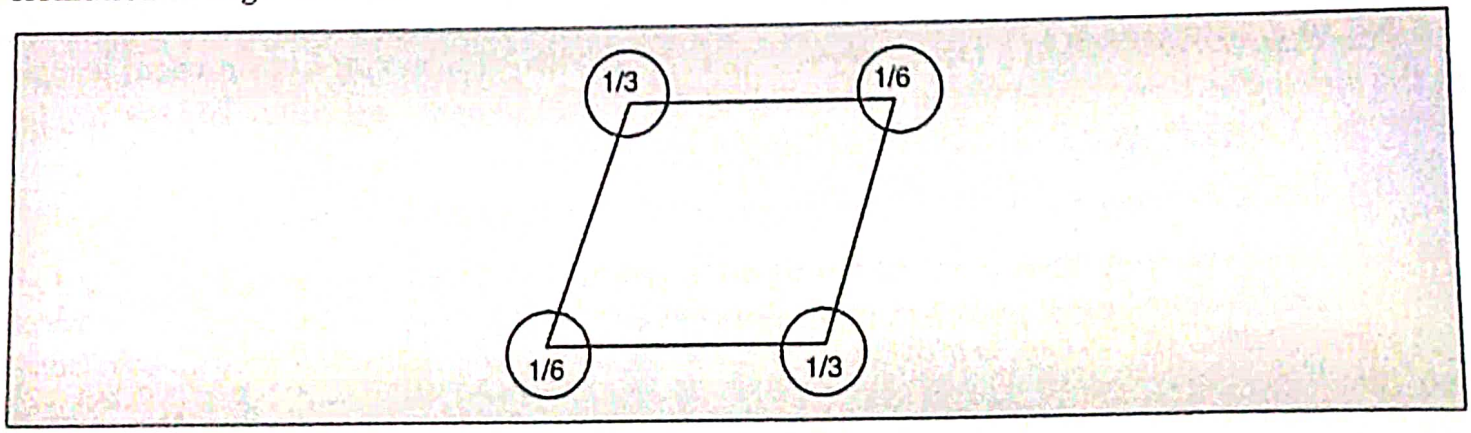


Fig. 1.8.

1.10

$\frac{1}{3}+\frac{1}{6}+\frac{1}{3}+\frac{1}{6}=1$, this corresponds to a primitive unit cell. On the other hand, there is another one lattice point in side the unit cell and it sums to be two lattice points (Fig. 1.0) in making this unit cell. The unit cells which possess more than one lattice point is called non-primitive unit cell.

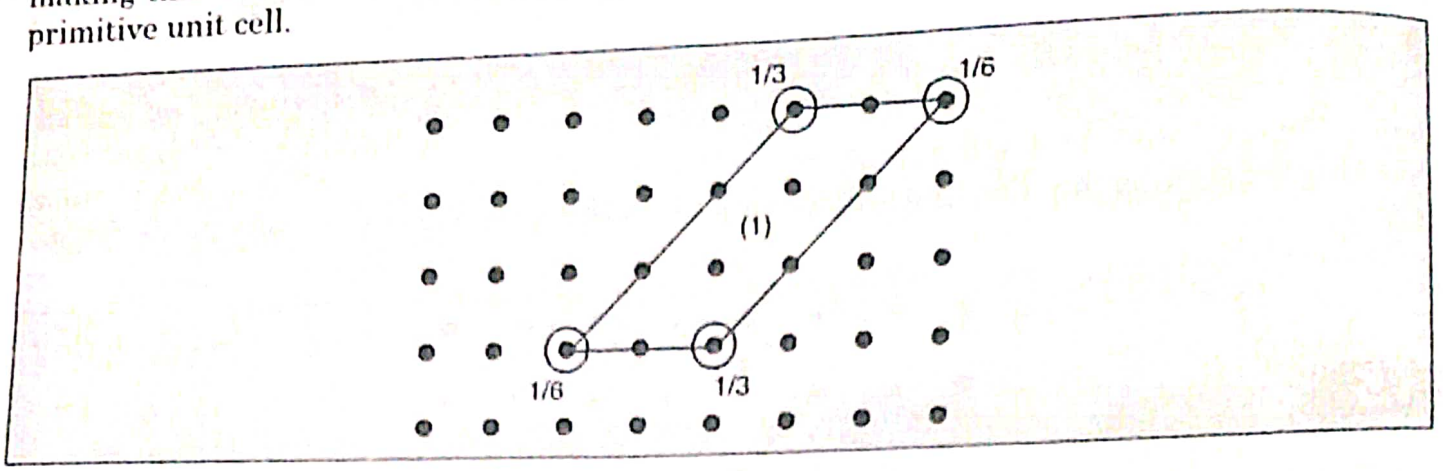


Fig. 1.9.

Total contributing lattice points in one unit cell formation in $\frac{1}{3}+\frac{1}{6}+\frac{1}{3}+\frac{1}{6}+1=2$, this corresponds to a non primitive unit cell.

Point to Remember

If there is a lattice point at the edge of a cell and thus shared with another cell, it is only counted as half. Similarly, a point located on the corner of a cube is shared by 8 cubes and would count with 1/8.

The main property of the primitive cell is that its area is minimum in two dimensions and volume is minimum in three dimensions. There are many ways of choosing the primitive unit cell but for a given lattice, area or volume of all the primitive cells is same.

Primitive Basis : The basis associated with a lattice point of primitive cell is known as primitive basis. Minimum number of atoms are there in the primitive basis. For primitive basis, the unit cell is called the primitive cell. It contains only one lattice point. For non primitive basis, the unit cell is a multiple cell and it contains more than one lattice points.

Wigner-Seitz Cell : A special type of primitive cell is called a Wigner-Seitz cell. When the lattice points are not at the corners of a primitive cell, then the Wigner-Seitz cell is another way of choosing the primitive cell.

The Wigner-Seitz cell of a lattice point is defined as the volume which encloses all points in the space which are closer to the particular lattice points than in any other. The method to draw the Wigner-Seitz cell.

(i) Draw the lines to connect a given lattice point to all nearby lattice points.

(ii) Draw the new lines passing through midpoints and perpendicular to these lines in two dimensions or planes in three dimensions.

(iii) The smallest area in two dimensions or the smallest volume enclosed by normal lines or planes is called the Wigner-Seitz cell (Fig. 1.10).

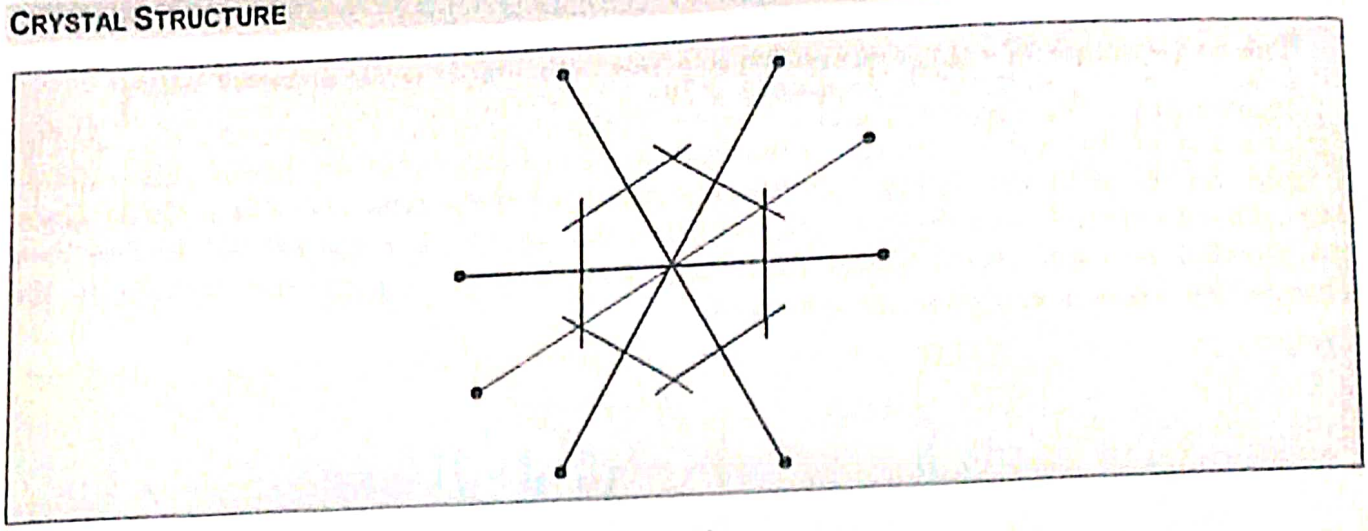


Fig. 1.10.

1.5 LATTICE WITH A BASIS

From geometrical considerations, a regular periodic arrangement of particles can be explained with the help of a translation. Fig. 1.3 showed a lattice obtained with the help of translation of particle along two dimensions. A lattice built up with the help of translation of any site along the three directions is called a **Bravais lattice**, named after a French Physicist Auguste Bravais (1811-1863). The lattice sites are the apexes of the cell occupied by identical atoms or groups of atoms and are so equivalent.

Not every type of lattice may be obtained by translation of a single site Fig. 1.11 shows a two dimensional lattice with a general type basis. It is impossible to obtain a unit cell of such a lattice in terms of a single-site unit cell. Such a lattice may be thought as comprising of two Bravais lattices, 1 and 2 each obtained by the basis vectors $\vec{a}$ and $\vec{b}$ and inserted into each other.

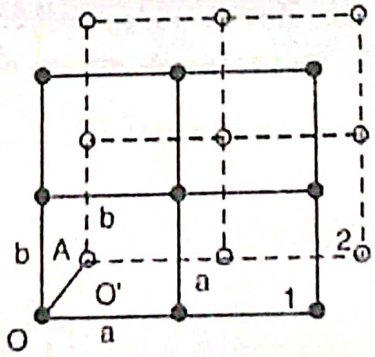


Fig. 1.11.

The relative displacement of the lattice is described by an additional basis vector $\vec{A}$. There is no fixed number of such basis vectors, it is arbitrary.

The lattice of the type shown in Fig. 1.11 is known as **lattice with a basis**. It may be obtained with the help of the same translations as can be used to obtain any of the Bravais lattices that make it up. Here, we translate not one site but many sites–the basis defined by the totality of the basis vectors. Hence the two dimensional lattice shown in Fig. 1.11 may be described by a translation of the basis obtained by two sites O and O.'

1.12 The best example of a three dimensional lattice with a basis is the diamond lattice.

Symmetry : The regularity and symmetry is the most obvious feature of a crystal. The surrounding of the crystal remain unchanged due to periodicity of the lattice point. Let us consider a cube as shown in Fig. 1.12 in which the base of the cube is the face ABCD. Here, four faces are vertical and they intersect at four lines AE, CG, DH and BF. All the four lines are parallel to each other. These four faces form a zone and an axis parallel to the intersecting edges is known as the zone axis.

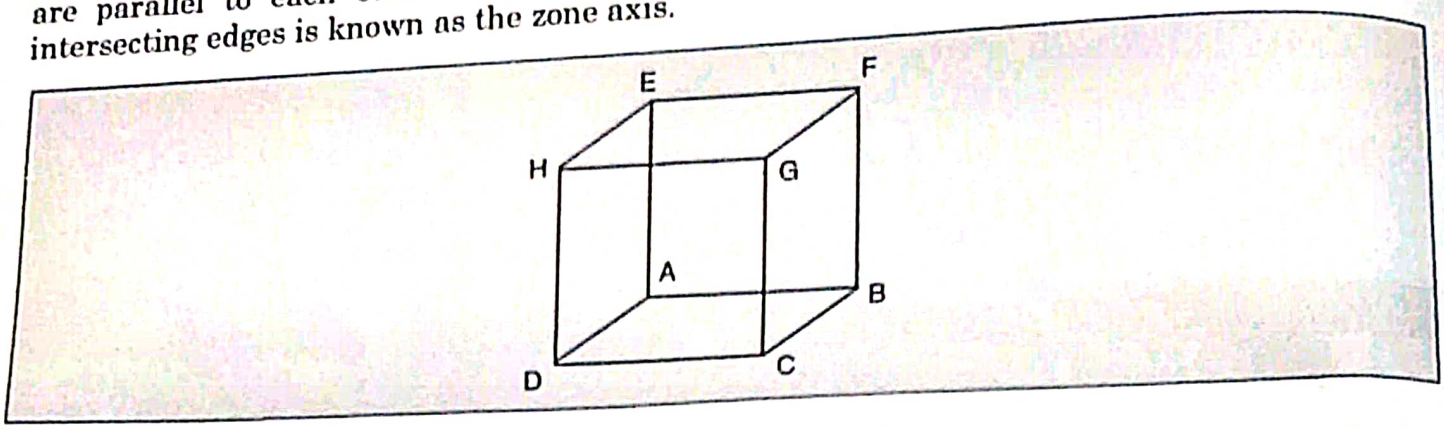


Fig. 1.12.

On rotating a cube about a zone axis passing through the centre of the cube, a rotation through 90° brings the cube in a similar position *i.e.* in a position same as that of the original position. This rotation axis is known as the axis of the symmetry. In general if a rotation of $2\pi/n$ about an axis brings a solid figure into a congruent *i.e.* similar position, then the axis is called n-fold axis. A rotation through 360° for any crystal brings the crystal back to its original position. This type of an axis is known as identity axis. When $n = 2$, the crystal is said to be in two fold symmetry and the axis is called diad axis. When $n = 3$, the crystal is said to be in three fold symmetry and the axis is called a triad. For $n = 4$ and 6. The axis is called tetrad and hexad respectively. The integer n is called the multiplicity of the axis.

Theoretically, n can have any value say $n = 1, 2, 3, 4, 5, 6, 7, 8$ etc. for any solid. Most of these solids are glass, wood, clay etc. But in the case of crystalline solid n can have only five values *i.e.* $n = 1, 2, 3, 4, 6$. The crystalline solids do not show a five fold symmetry or higher than six. To prove this consider the combination of a n-fold axis x_0 with a translation $\vec{p}$ as shown in Fig. 1.13.

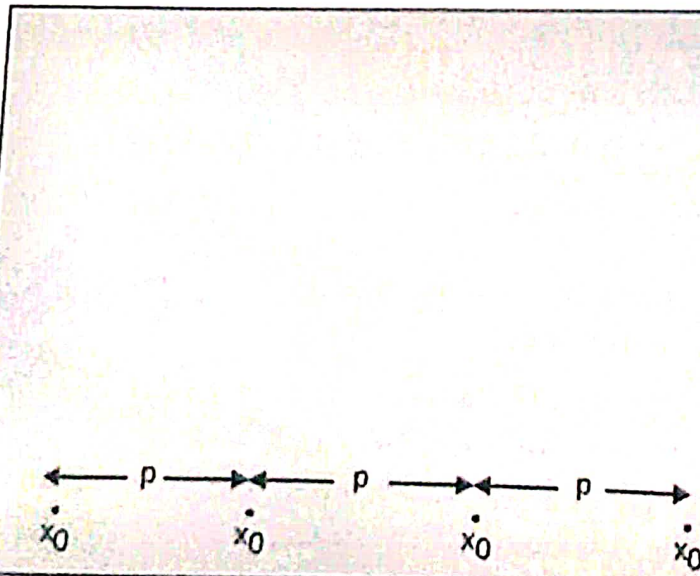


Fig. 1.13.

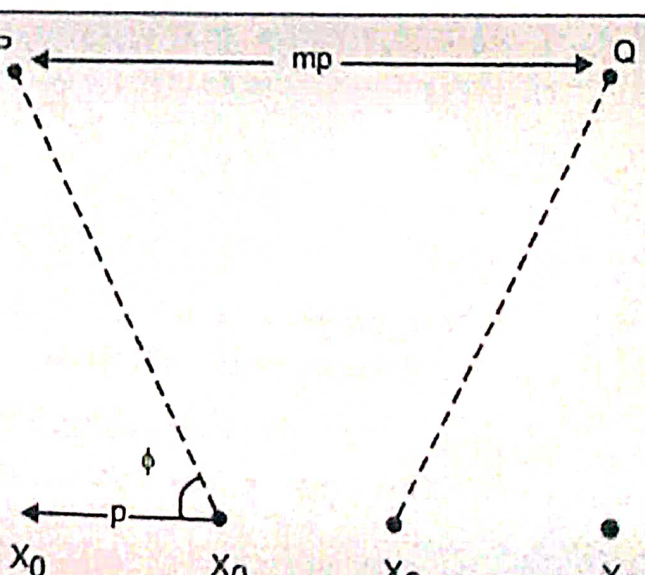


Fig. 1.14.

A lattice is said to possess the rotational symmetry about an axis if the rotation of the lattice about that axis by some angle ϕ leaves it invariant. A rotation axis will repeat the translation after a rotation through $(2\pi/n)$. Using this linear array, two rotations through $(2\pi/n)$ will produce new lattice points P and Q as shown in Fig. 1.14. Let the distance between the two points P and Q be mp. Let us determine n geometrically from Fig. 1.14.

$$mp = p + 2p\cos\phi$$

or
$$m = 1 + 2\cos\phi$$

$$(m - 1) = 2\cos\phi$$

Let $(m - 1)$ be another integer say n', then we have

$$\cos\phi = \frac{n'}{2}$$

The above equation can be satisfied by

$n' = \pm 2, \pm 1, 0$ or $\phi = 180°, 120°, 90°, 60°, 360°$

which correspond to $n = 2, 3, 4, 6, 1$. Therefore, we conclude that the five fold symmetry is not possible. Similarly seven fold, eight fold etc. rotation axes are not possible in lattice. A single molecule properly designed can have any fold rotation axes. We can design a unit cell which has five fold symmetry as shown in Fig. 1.15 but we can not expect the lattice to have five-fold symmetry, because it is not possible to fill up all the space by the unit cell of pentagons. Also heptagon and octagon cannot fill the entire space and so the lattice cannot have seven fold and eight fold rotational axes.

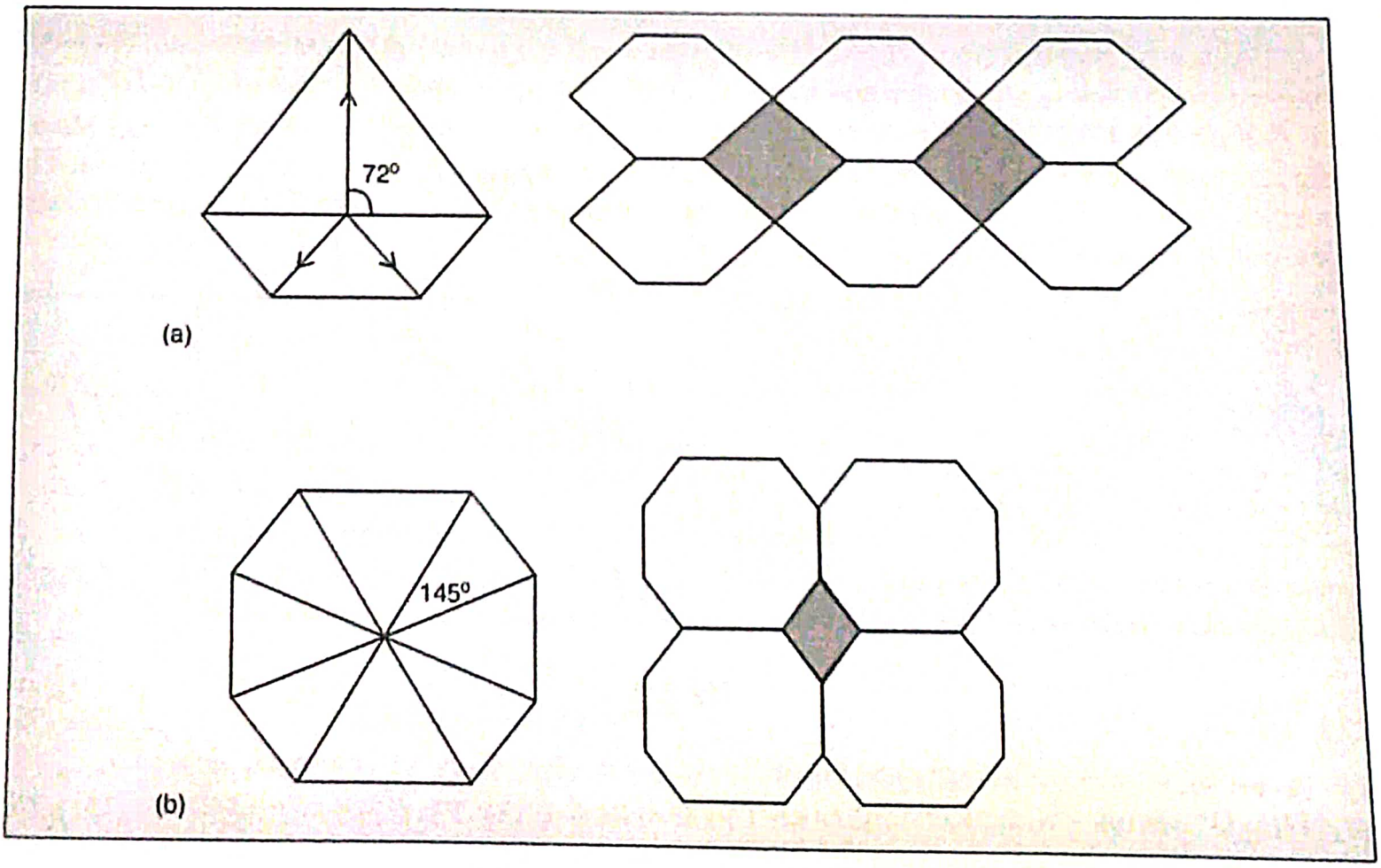


Fig. 1.15.

The shaded portions in Fig. 1.15 (a) are the empty spaces left after placing pentagons in adjacent where pentagon cannot be adjusted. Also, in Fig. 1.15 (b), octagon cannot be adjusted. Hence, five fold and eight fold symmetries do not exist in crystals.

Quasi Crystals : Some crystalline like solids, which do not have regular crystal like pattern but posses quasi periodicity and behave like crystals are called quasi periodic crystals or simply quasi-crystals. It is a crystal which has an ordered structure but is not periodic. This pattern can continuously fill all available space but it does not have translational symmetry. Quasi crystals exist with five fold symmetry.

Bilateral Symmetry : If a plane or a unit cell divides it into two equal halves in such a way that the one half is the reflection of the other half along. The plane, then the plane is referred as a plane of symmetry. This kind of symmetry is called a bilateral symmetry. In a cube, there are three planes of symmetry as shown in Fig. 1.16.

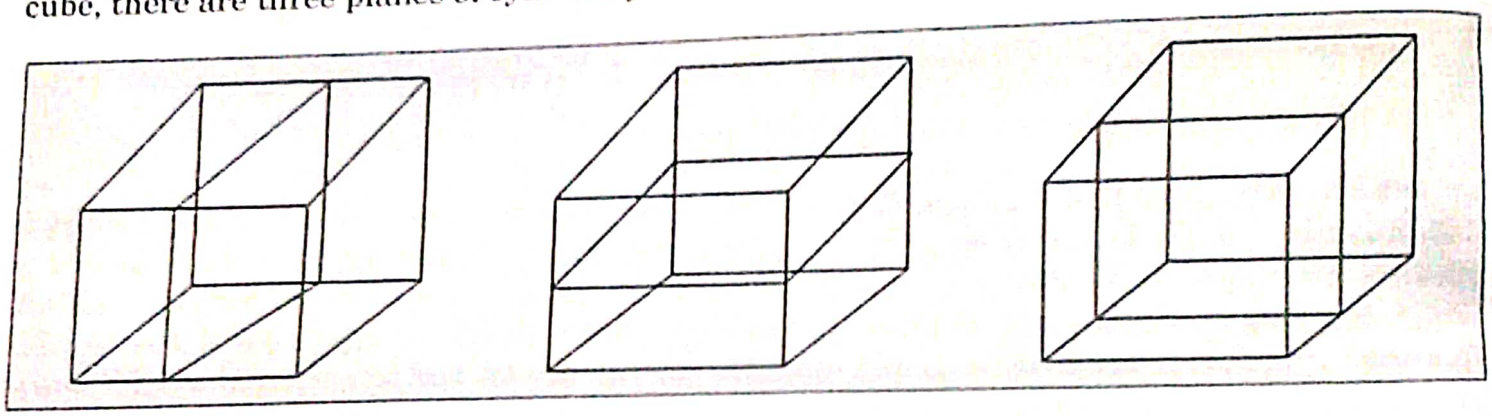


Fig. 1.16.

Centre of Symmetry : The centre of symmetry is a point in the crystal such that if a line is traced from any point on the figure through this point and produced an equal distance on the other side of the centre of symmetry, then it meets an identical point. Fig. 1.17 shows six diagonal planes of symmetry centre of symmetry is also known as inversion centre. For every lattice point in the crystal position at distance r then another lattice point is also present at distance $-r$.

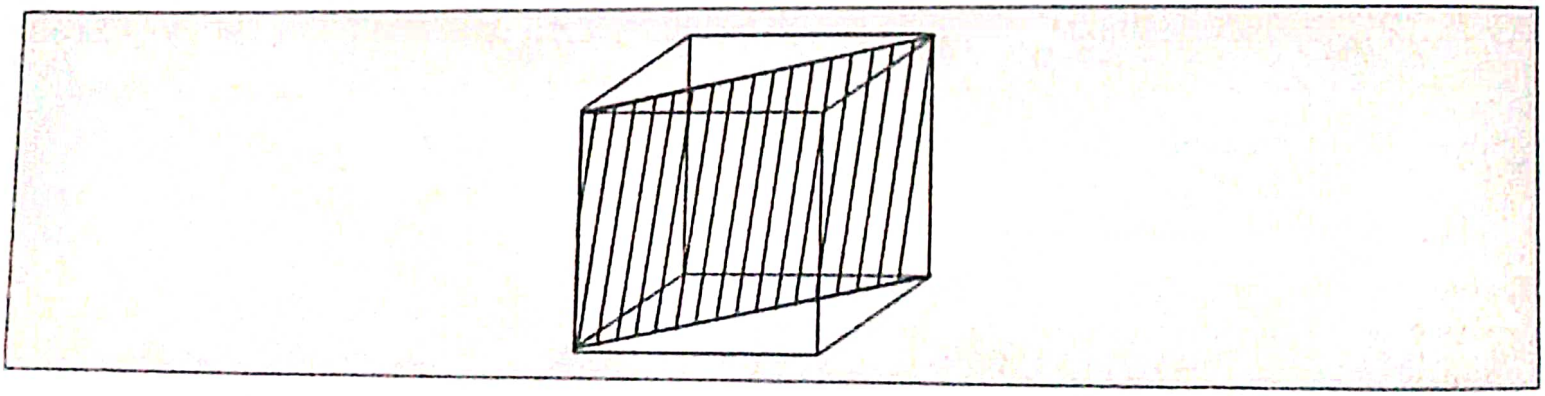


Fig. 1.17.

A sense of a symmetry is a powerful tool for the study of internal structure of the crystals. Of course an ideal crystal cannot be obtained there are always deviations from ideal conditions. These deviations from the ideal crystals are due to following two reasons.

(i) There are deviations at the surface where the periodicity condition breaks down.

(ii) There are deviations due to dislocations, impurities and imperfections in the interior structure.

Inspite of the deviations, we prefer to use symmetry to classify the crystals.

1.6 TYPES OF LATTICES

Bravais in 1848 was the first to position the structure less points in space such that all the points have similar surroundings. These lattices known after his name are five lattice types or unit cells in two dimensions, fourteen in three dimensions and sixty four in four dimensions.

Two Dimensional Bravais Lattices : On the basis of rotational symmetry we can classify two dimensional lattices as following :

Type of Lattice	Rotational Symmetry	Relation between the crystal axes
Oblique	2-fold	$a \neq b$, ϕ arbitrary
Square	4-fold	$a = b$, $\phi = 90°$
Hexagonal	6-fold	$a = b$, $\phi = 120°$

There are additional two sets of mirror planes in the square and hexagonal lattices. The oblique lattices in general do not possess reflection symmetry. In two dimensions, two more additional lattice types (i) primitive rectangular and (ii) centered rectangular occur. Hence, in all there are five distinct types of lattice in two dimensions. They are listed as follows :

S.No.	Lattice	Conventional unit cell	Crystal axes	System	Point group
1.	Oblique	Parallelogram	$a \neq b$, $\phi = 90°$	Oblique	1, 2
2.	Square	Square	$a = b$, $\phi = 90°$	Square	4, 4 mm
3.	Hexagonal	60° rhombus	$a = b$, $\phi = 120°$	Hexagonal	3, 3 m, 6 mm
4.	Primitive rectangular	Rectangle	$a \neq b$, $\phi = 90°$	Rectangle	1 m, 2 mm
5.	Centered rectangular	Rectangle	$a \neq b$, $\phi = 90°$	Rectangle	1 m, 2 mm

The total symmetry of space about a point is found by a collection of symmetry elements at that point. A **point group** is the group of set of symmetry operations at a point. As there are two possible point groups associated with a rotation axis with or without reflection symmetry, there are, hence a total of ten possible point groups allowed in two dimensions. These are

1, 1 m, 2, 2 mm, 4, 4 mm, 3, 3 mm, 6, 6 mm

In the point groups mentioned above, the first symbol signifies to the rotations about the point, for example the point group 2 refers to 2-fold rotations. The second symbol signifies to the reflection lines parallel to the rotation axis. These ten mentioned above are called crystallographic point groups and are shown in Fig. 1.18.

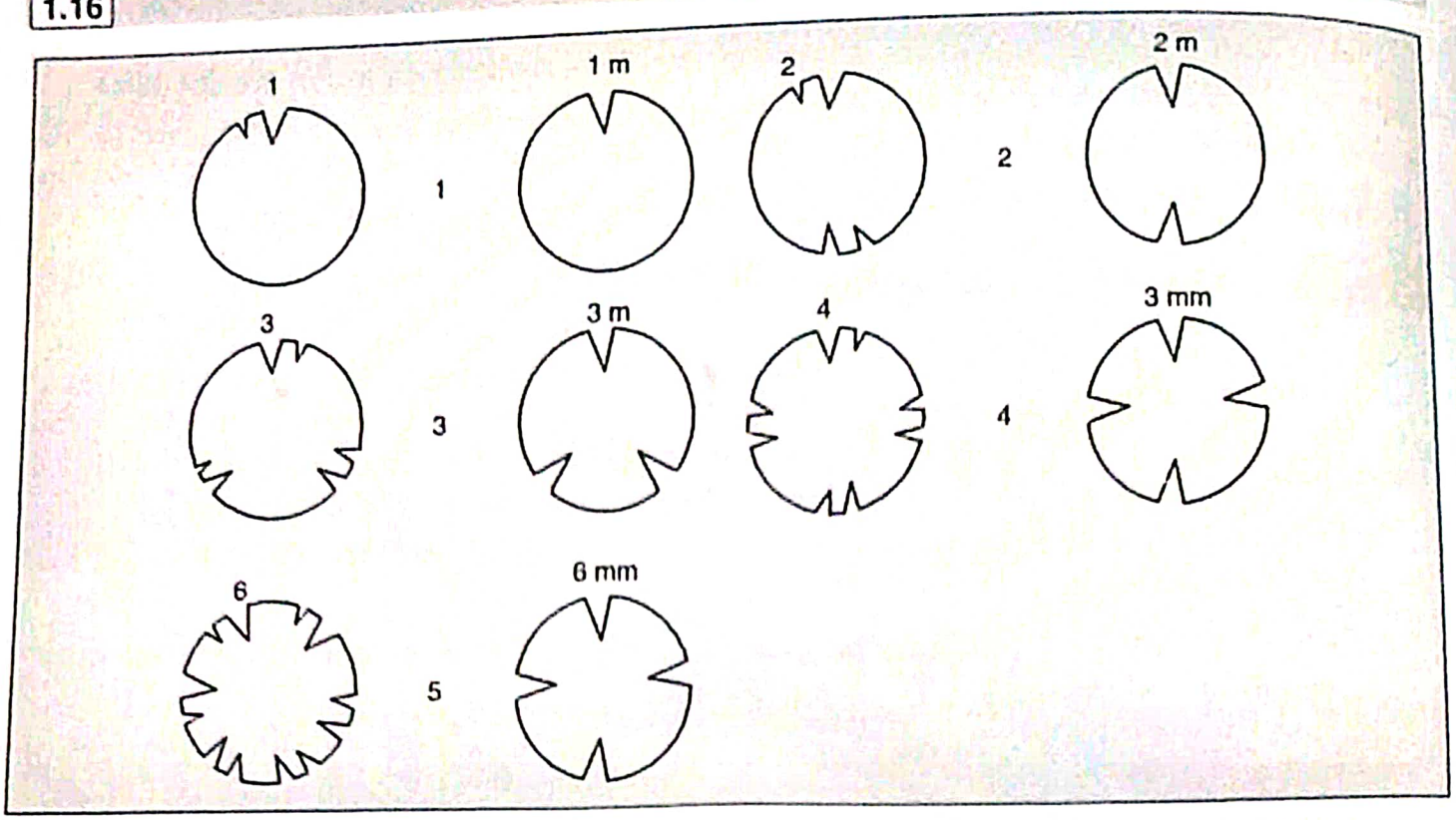


Fig. 1.18.

Now consider an oblique lattice as shown in Fig. 1.19 with translational vectors $\vec{a}$ and $\vec{b}$. We want to study the result of relation between $\vec{a}$ and $\vec{b}$ when one imposes reflection symmetry on this lattice.

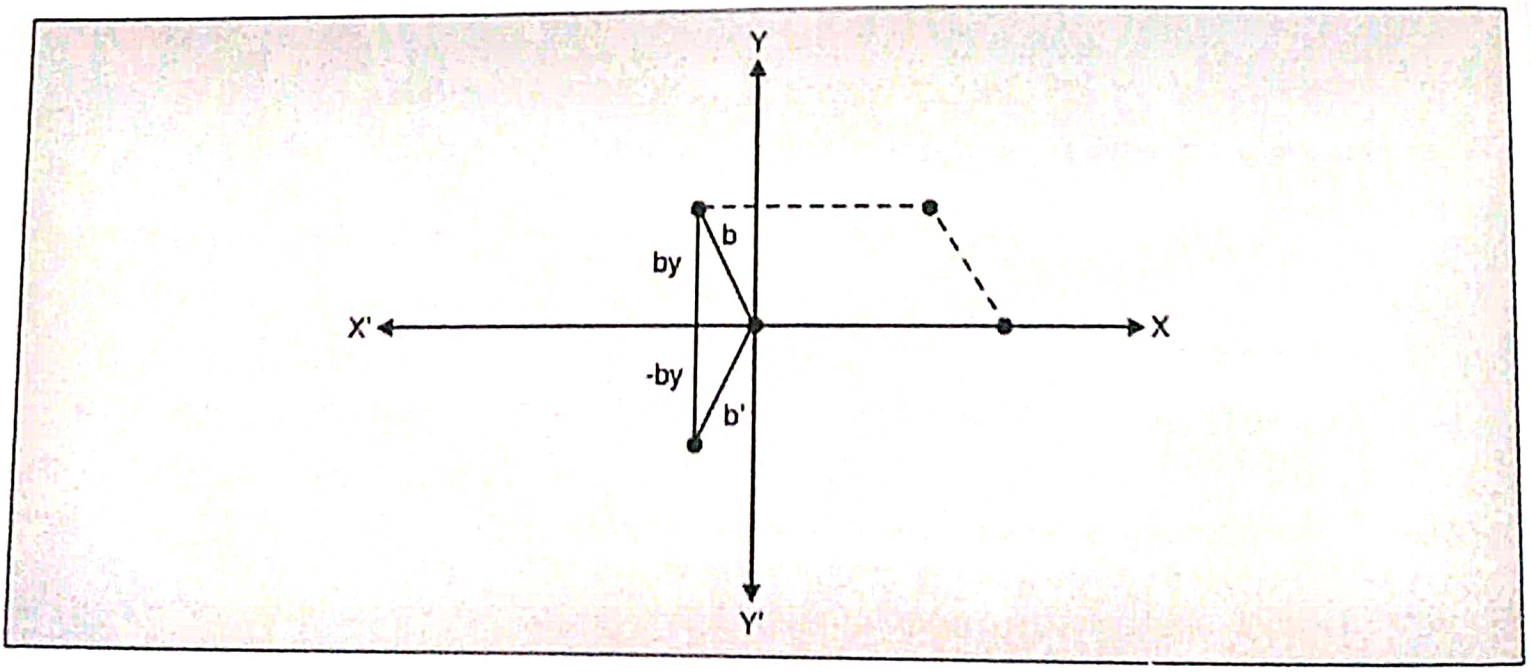


Fig. 1.19.

The vectors $\vec{a}$ and $\vec{b}$ can be expressed with reference to cartesian coordinate system as

$$\vec{a} = a_x \hat{i}$$

$$\vec{b} = b_x \hat{i} + b_y \hat{j}$$

For simplicity, assume X-axis to be a reflection line so that the reflection of lattice in this reflection line will give new vectors $\vec{a'}$ and $\vec{b'}$ such that

$$\vec{a'} = a_x \hat{i}$$

$$\vec{b'} = b_x \hat{i} - b_y \hat{j}$$

For the lattice to be invariant under the reflection, $\vec{a'}$ and $\vec{b'}$ must also be lattice vectors. In other words, they must be of the form $n_1 \vec{a} + n_2 \vec{b}$ where n_1 and n_2 are integers.

As $\vec{a'} = \vec{a}$ and so we have to set

$$\vec{b'} = n_1 \vec{a} + n_2 \vec{b}$$

$$= n_1 b_x \hat{i} + n_2 (b_x \hat{i} + b_y \hat{j})$$

Equating coefficients of $\hat{i}$ and $\hat{j}$ in the above equations, we have

$$b_x = n_1 a_x + n_2 b_x$$

$$-b_y = n_2 b_y$$

and $$n_2 = -1$$

Hence, $$b_x = \frac{n_1 a_x}{2}$$

and b_y is arbitrary. If $n_1 = 0$ and $b_x = 0$ can easily be verified for all even n_1 and we have the primitive lattice. The above equations have a solution if $n_1 = 1$, $b_x = \frac{a_x}{2}$ and $2\, b_x = a_x$, thus a primitive translational vectors for a lattice with mirror symmetry becomes as

$$\vec{a} = a \hat{i}$$

$$\vec{b} = \frac{1}{2} a \hat{i} \; b_y \hat{j}$$

The above choice gives a centered rectangular lattice which can be verified for all odd n_1.

The five lattice types discussed so far–oblique, primitive rectangular, centered rectangular, square and hexagonal are known as the five Bravais lattices and are shown in Fig. 1.20.

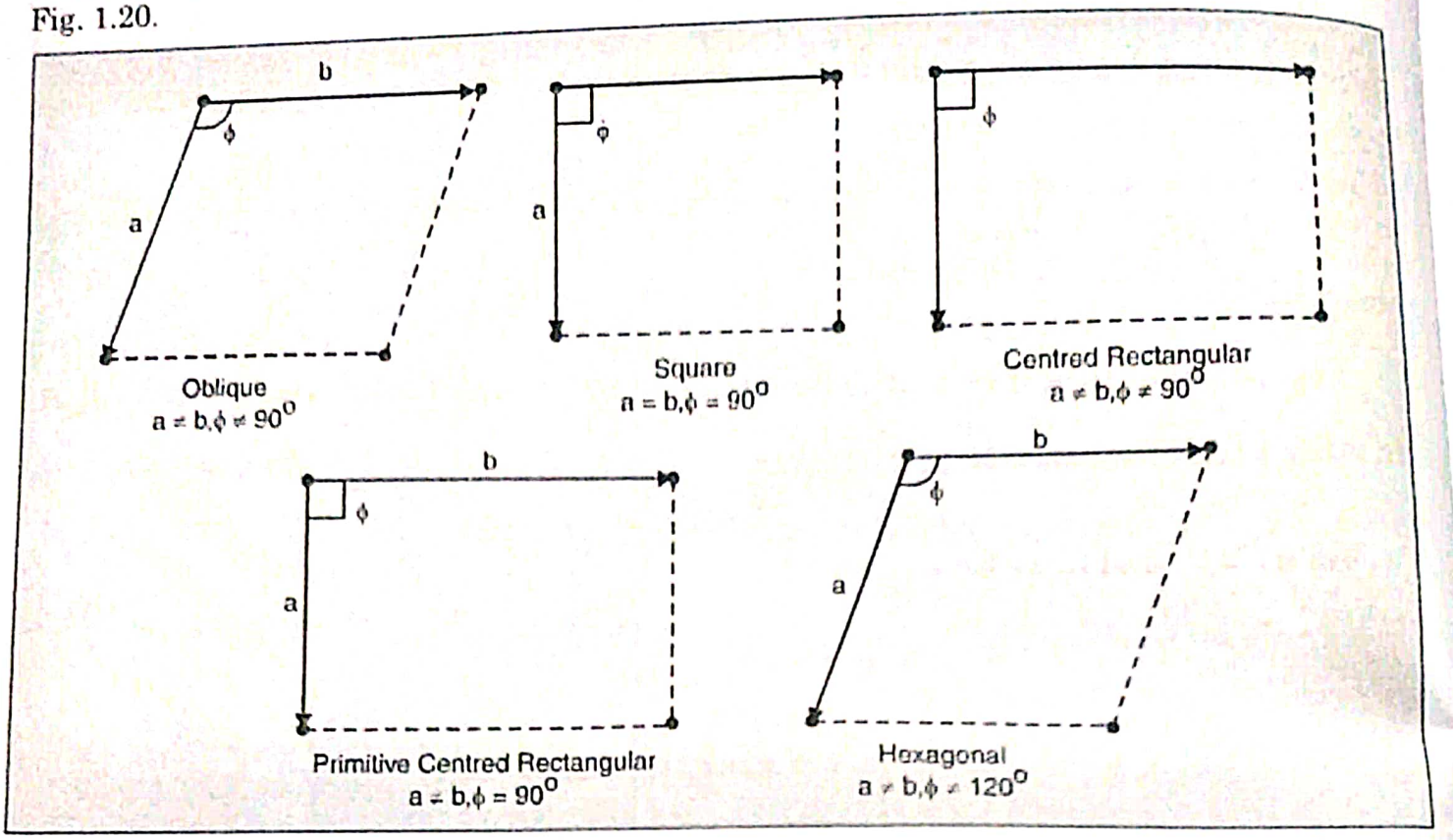


Fig. 1.20.

There is one more way of classification of lattices by crystal systems in which the primitive and centered rectangular lattices are considered as belonging to a single rectangular system. In this way, there will be four crystal systems in two dimensions–oblique, rectangular, square and hexagonal.

Point to Remember

It is the point symmetry of the basis that determines the types of lattice formed in the crystal.

Remember, to specify the symmetry of a crystal structure, we must consider the following aspects.

(i) there must be point symmetries at more than one location in a unit cell, and

(ii) there exists symmetry elements comprising of combined point and translation operations.

The collection of all the symmetry elements of crystal structure is known as the **space group.** The space group is determined by the lattice and the basis. The repetitive pattern of the symmetry elements of the crystal structure is specified by the space group. In two dimensions there are seventeen possible space groups and are known as **plane patterns.**

Three Dimensional Bravais Lattices : In three dimensions there are seven crystal systems–triclinic, monoclinic, cubic, tetragonal, orthorhombic, triogonal and hexagonal.

The cubic and hexagonal lattices are close analogues of the square and hexagonal lattices n two dimensions. The triclinic lattice in three dimensions is analogue to the oblique and the

orthorhombic is analogous to the rectangular lattice in two dimensions. The monoclinic lattices have some oblique and some rectangular properties.

The tetragonal lattices are partly square and partly rectangular. The trigonal lattice has some aspects of centered rectangular lattice. Thus, we can think of some comparison between the two-dimensional and the three dimensional lattices.

The 14 Bravais lattices are shown in Fig. 1.21 and table gives the seven systems and fourteen lattices.

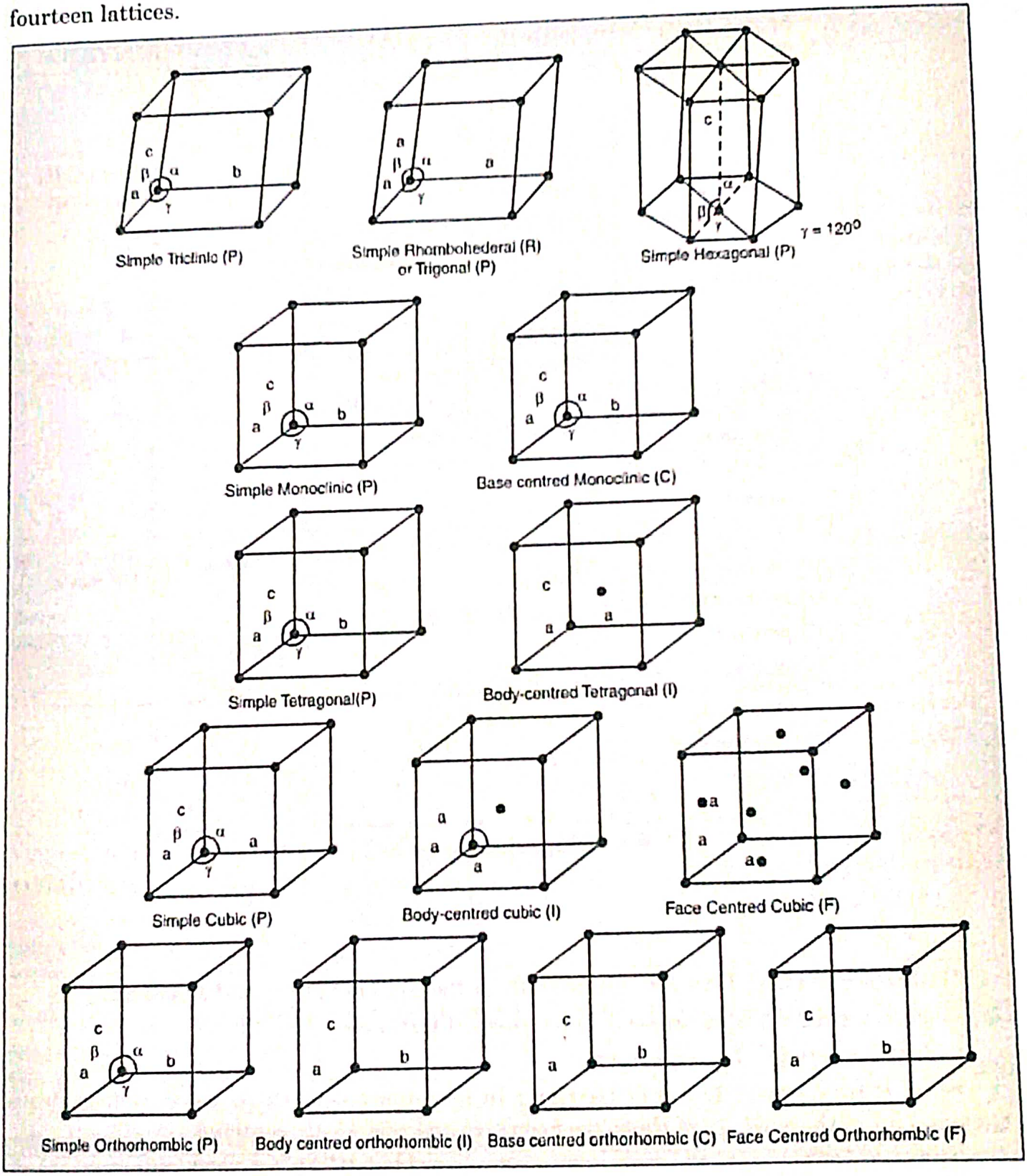


Fig. 1.21.

Crystal system	Characteristic symmetry elements	Bravais lattice and its symbol	Restrictions on conventional unit cell axes and angles	Length and angles to be specified	Examples
Triclinic	None	1. P (simple)	$a \neq b \neq c$	a, b, c	$FeSO_4, 5H_2O$
			$\alpha \neq \beta \neq \gamma \neq 90°$	α, β, γ	$CaS_2O_3.6H_2O$
Mono-clinic	One two fold	1. P (simple)	$a \neq b \neq c$	a, b, c	$Li_2SO_4.H_2O$
	rotation axis 2/m	2. Base centered (C)	$\alpha = \gamma = 90° \neq \beta$	β	$Na_2B_4O_7.10H_2O$ (Borax)
Ortho-rhombic	Three mutually Perpendicular 2-fold rotation axes mmm	1. Simple (P) 2. Base centered 3. Body centered (I) 4. Face centered (F)	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$ (orthorhomb)	a, b, c	$PbSO_4C_6H_2(NO_2)_4OH$
Tetragonal	One 4-fold rotation axis or a 4 fold rotation inversion axis $\frac{4}{nm}$	1. Simple (P) 2. Body centered (I)	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$ (right square prism)	a, c	In MgCl, Sn
Cubic	Four 3-fold rotation axes (cube-diagonal m 3m	1. Simple (P) 2. Body centered (I) 3. Face centered (F)	$a = b = c$ $\alpha = \beta = \gamma = 90°$	a	Au, Cu, Ag, Fe, NaCl. (Most metals and their alloys)
Hexagonal	One 6-fold rotation axis 6/mmm	1. Simple (P)	$a = b \neq c$ $\lambda = \beta = 90°$ $\gamma = 120°$	a, c	$Be_3Al_2(Si_6O_{18})$ Be, Mg, Zn, Cd.
Trigonal (Rhombohedral)	One 3-fold rotation axis	1. Simple (R)	$a = b = c$ $\alpha = \beta = \gamma$ $<120°, \neq 90°$ (right Prism)	a α	$CaCO_3$ $MgSO_4.6H_2O$

*Lattice symbols P–Primitive (atoms only at the corners of the parallelepipedon)

C–Base centered (extra atoms at the centers of the base)

I–Body centered F–Face-centered

Four Dimensional Bravais Lattice : In four dimensions there are sixty four Bravais lattices. Out of these 64, 23 of them are primitive and rest 41 are centered.

(i) Triclinic crystals have three axes of unequal length. No two of the three axes are at right angles to each other. The faces of these crystals are all different and do not meet at

right angles and has no symmetry along any axis. Triclinic unit cell can be visualised if we apply stress on the diagonally opposite corners of the empty carton of unequal sides (Fig. 1.22).

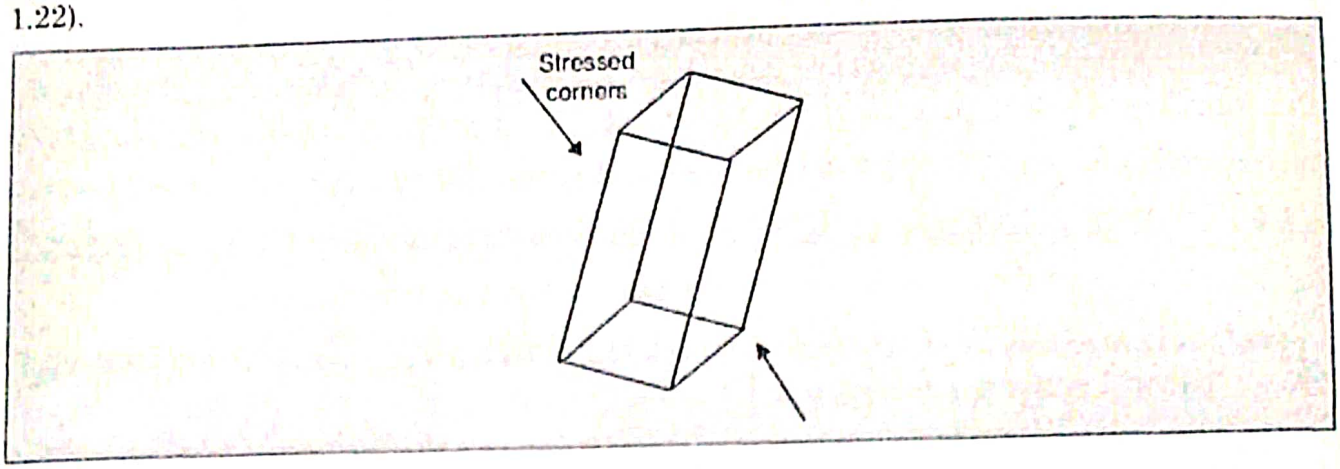


Fig. 1.22.

(ii) Monoclinic crystals have three axes of different lengths. In this crystal, one of the axes is at right angles to the other but the other two axes are not at right angles to each other. Monoclinic crystal has two fold symmetry only in one dimension. This gives rise to the parallelepiped lattice with stress on two opposite edges. This can be visualised if we take the empty carton with three sides of unequal length and we press the two opposite edges as shown in Fig. 1.23.

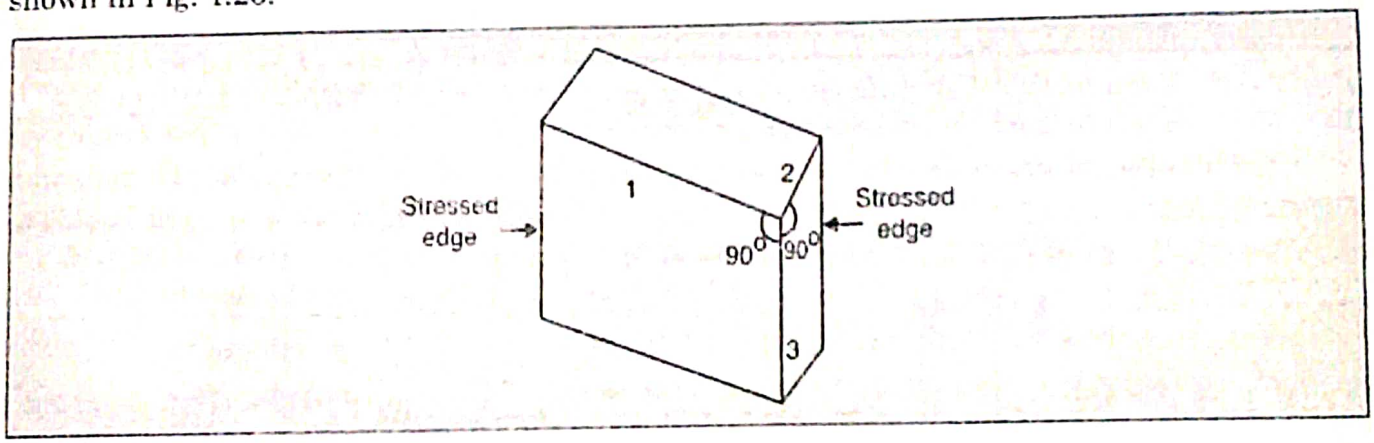


Fig. 1.23.

(iii) Orthorhombic crystals have three axes of unequal length that intersect at right angles. They have two fold symmetry along three mutually perpendicular directions. The cell is orthogonal because all the three axes are mutually perpendicular. It can be visualised by taking a carton with three sides mutually perpendicular but of unequal lengths as shown in Fig. 1.24.

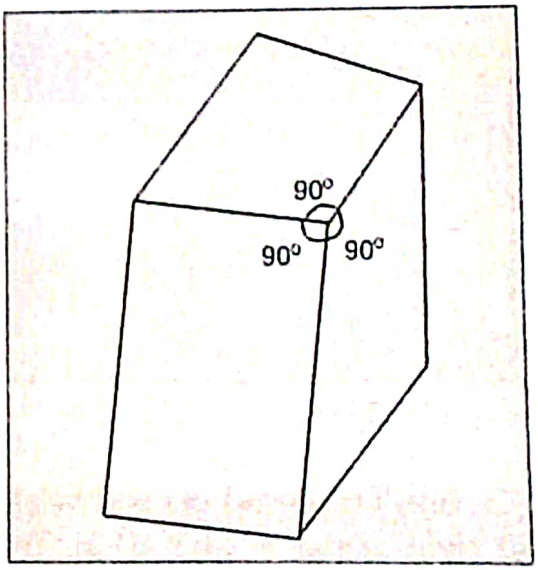


Fig. 1.24.

(iv) Tetragonal crystals have the three axes at right angle to each other. Two of the axes are of equal length. In tetragonal lattice faces are rectangular and the top and bottom are square as shown in Fig. 1.25. Tetragonal crystals have four fold symmetry. Carton with three sides mutually perpendicular with two sides equal gives the tetragonal unit cell.

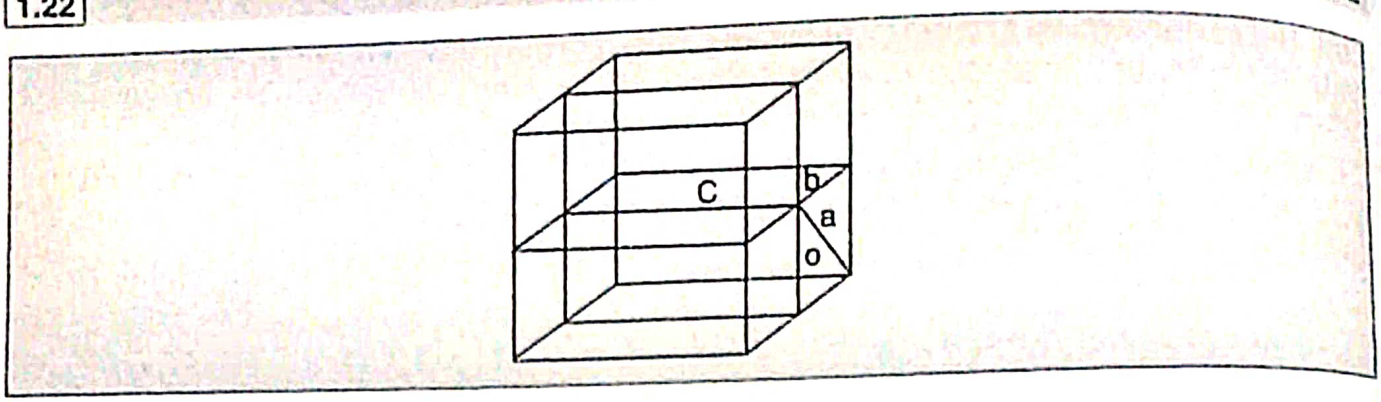


Fig. 1.25.

(v) Cubic crystals has three axes of same length which are at right angles to each other. It has a four-fold symmetry as shown in Fig. 1.26.

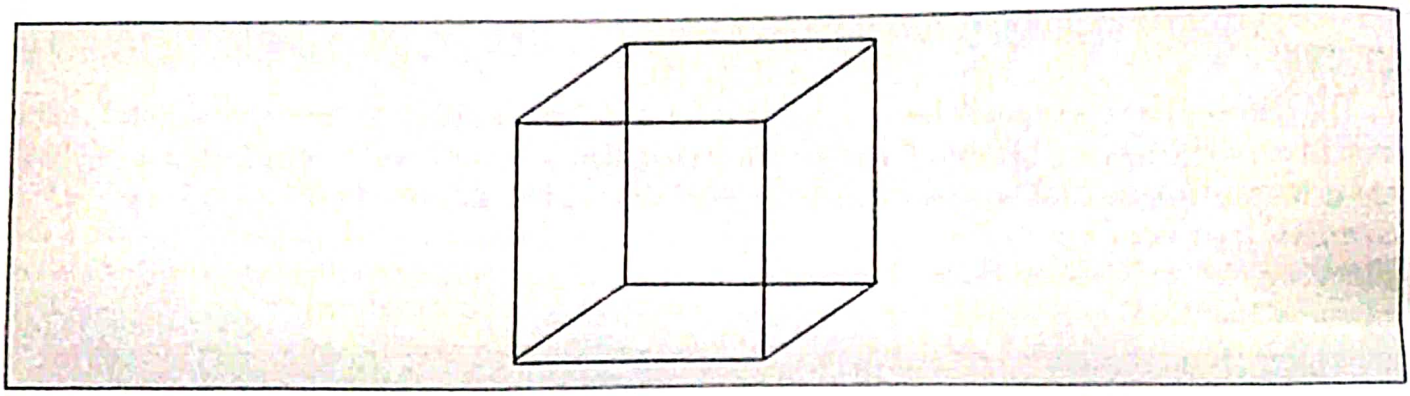


Fig. 1.26.

(vi) Hexagonal crystals has three axes in which two axes are of equal length lying in a horizontal plane with a 120° angle between one another. The third axes is at right angles to the others and may possess any length as shown in Fig. 1.27.

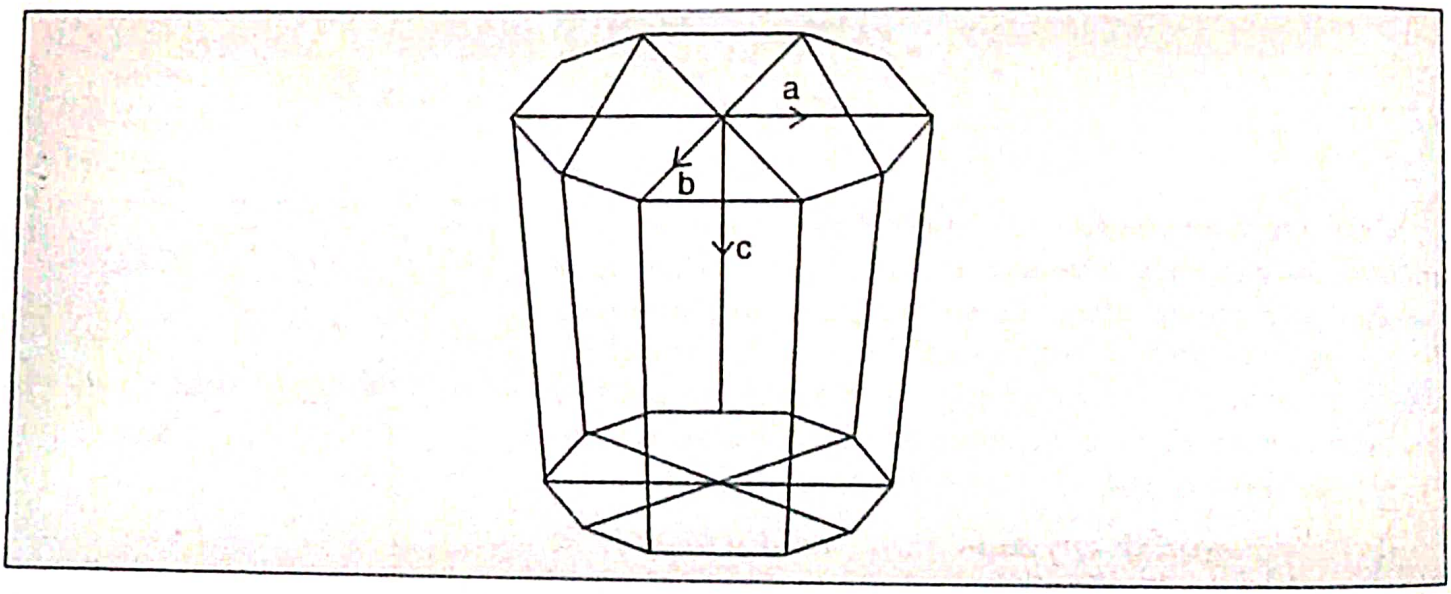


Fig. 1.27.

(vii)Triagonal crystal has three axes of equal length inclined at same angle but are not at right angles to each other. To visualise the triagonal lattice, take the cube and exert the pressure on diagonally opposite corners as shown in Fig. 1.28.

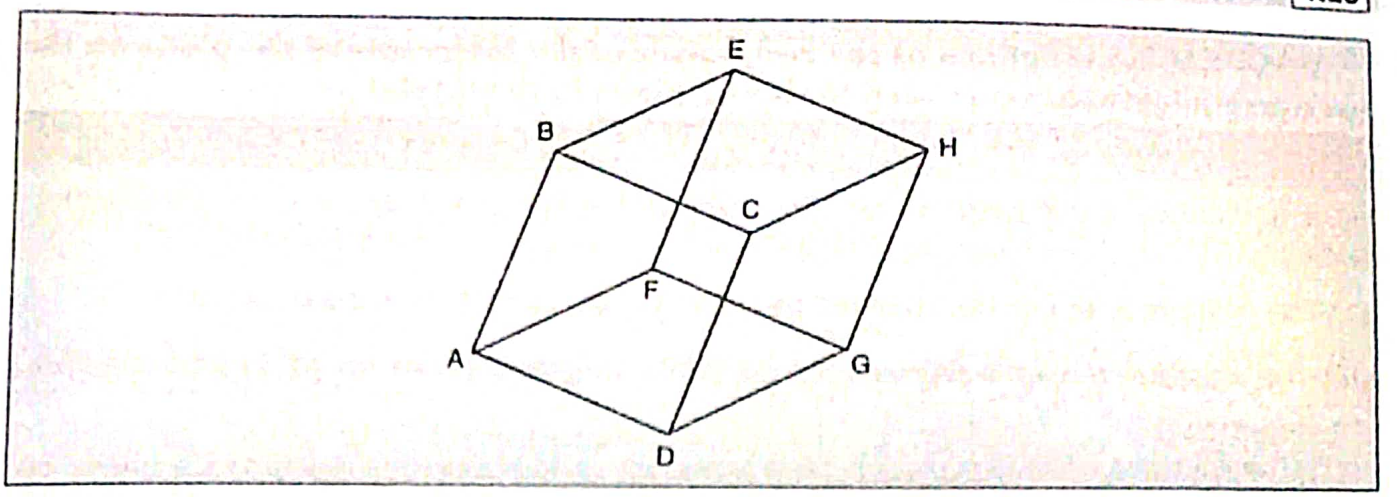


Fig. 1.28.

1.7 MILLER INDICES

William Hallowes Miller (1801-1880) a British mineralogist in 1839 introduced a system to represent a crystal plane or direction. He introduced a set of three numbers to specify a plane in a crystal.

Point to Remember

Miller indices are used to specify directions and planes in lattices or in crystals.

The properties of crystal depend on the inter-planer spacing and orientation due to which the crystals are anisotropic in nature. By anisotropic material we mean that the properties of these crystals change with different crystallographic orientations. So it becomes difficult to represent all planes on the plane of paper as for a given set of parallel planes the properties do not change. Therefore, if on replacing a set of parallel planes by a point in the space, then it becomes simple to draw all sets of planes and to analyse the properties of the crystals. Miller provided the method of replacing the set of parallel planes having same inter planer spacing and orientation by a point known as Miller indices. He introduced a set of three numbers to represent a plane in a crystal. The set of three numbers is known as Miller indices of the concerned plane.

Procedure of Finding Miller Indices : To find the Miller indices for a given plane, the following steps are to be followed :

(i) Find the intercepts of the plane along the axes X, Y and Z in terms of the lattice constants a, b and c.

(ii) The coefficients of the intercepts are noted separately.

(iii) Find the reciprocals of these numbers *i.e.* take the inverse.

(iv) The fractions are multiplied by a suitable number so that all fractions become integers. In other words, find the least common denominator (or multiplier) *i.e.* LCM and multiply each by this LCM,

(v) Write the integers in the form $(h\ k\ l)$. The notation $(h\ k\ l)$ denotes the set of all planes that are equivalent to $(h\ k\ l)$ by the symmetry of the lattice.

The three integers h, k and l are the Miller indices.

1.24

Miller Indices is defined as the reciprocals of the intercepts of the plane on the three crystallographic axes used to specify plane in the crystal.

Point to Remember

(i) A comma or a dot between any two numbers may be avoided while writing Miller Indices.

(ii) The positive X-axis is represented as (100), Y–axis as (010) and Z-axis as (001).

(iii) The negative X-axis is represented as $(\bar{1}00)$, negative Y-axis as $(0\bar{1}0)$ and negative Z-axis as $(00\bar{1})$.

(iv) The Miller Indices for a plane (101) is read as 'one zero one' and not as one hundred and one.

For an example, let us determine the Miller Indices of the plane shown in Fig. 1.29 by using the above procedure.

(i) The plane ABC shown in Fig. 1.29 makes intercepts $2a$, $3b$ and $2c$ along the X, Y and Z axes respectively.

(ii) Therefore the intercepts are $2a$, $3b$ and $2c$.

(iii) The coefficients of the intercepts are 2, 3 and 2

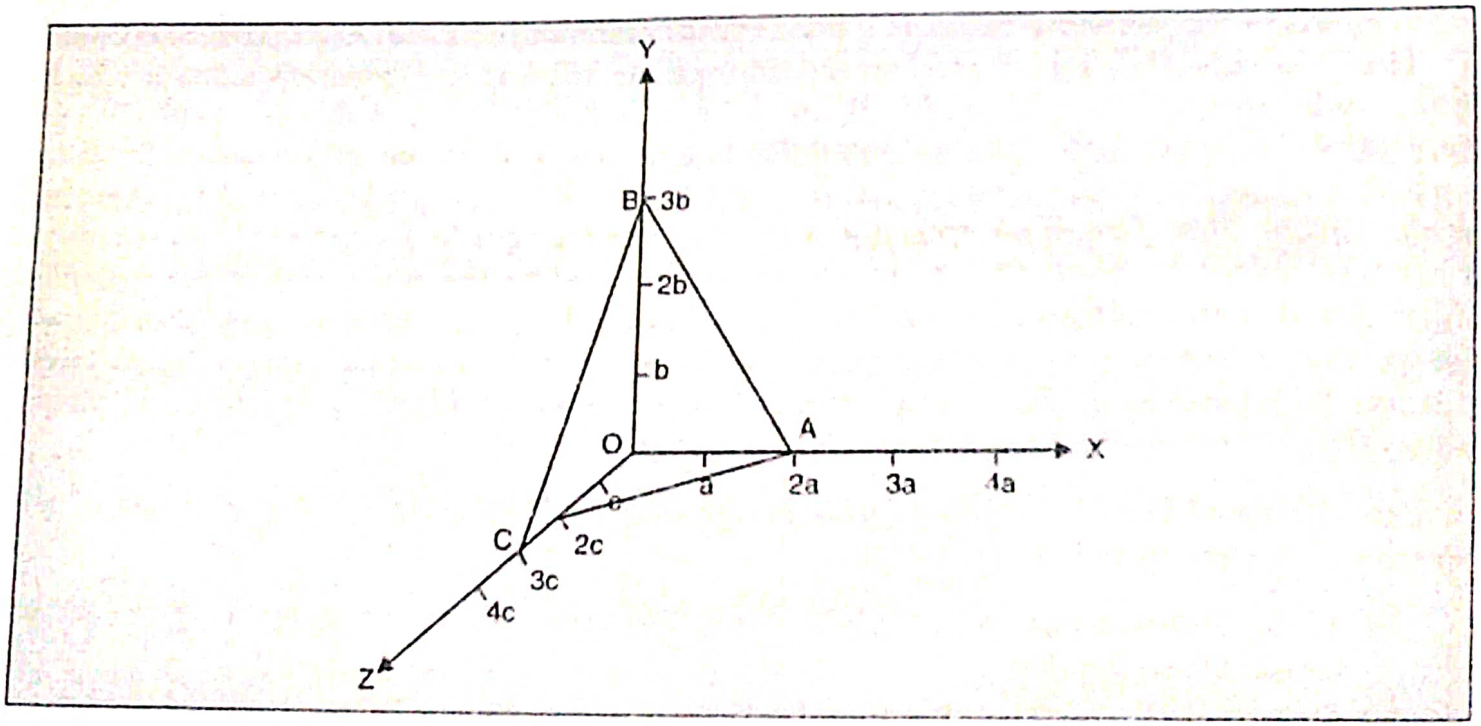


Fig. 1.29.

(iv) The inverse of the coefficients are $\frac{1}{2}$, $\frac{1}{3}$ and $\frac{1}{2}$.

(v) The LCM is 6.

(vi) Multiply the fractions by 6 so that they become integers as 3, 2 and 3.

(vii) The integers are written as (3 2 3) which represents the Miller indices of the given plane ABC.

Common Notations : Following are the common notations used in the study of Miller indices.

(i) (h, k, l) represents a lattice point. Here commas are used to signify the points.

(ii) Negative numbers and directions are represented with a bar on top of the number.

(iii) $[h\ k\ l]$ represents the direction.

(iv) $<h\ k\ l>$ represents a family of directions.

(v) $(h\ k\ l)$ represents a plane.

(vi) $\{h\ k\ l\}$ represents a family of plane.

(vii) For an intercept at infinity, the corresponding index is zero.

(viii) If a plane cuts an axis on the negative side of the origin, corresponding index is negative.

(ix) It is only the ratio of the indices which is important in the notation. The (6, 4, 6) planes are the same as (3 2 4) planes.

Point to Remember

All equally spaced parallel planes have same Miller indices.

Miller Indices of Some Important Planes in Cubic Crystal :

(i) The planes shown in Fig. 1.30 have intercepts $(1, \infty, \infty)$, $(2, \infty, \infty)$, $(3, \infty, \infty)$. These set of parallel planes have Miller indices (1 0 0)

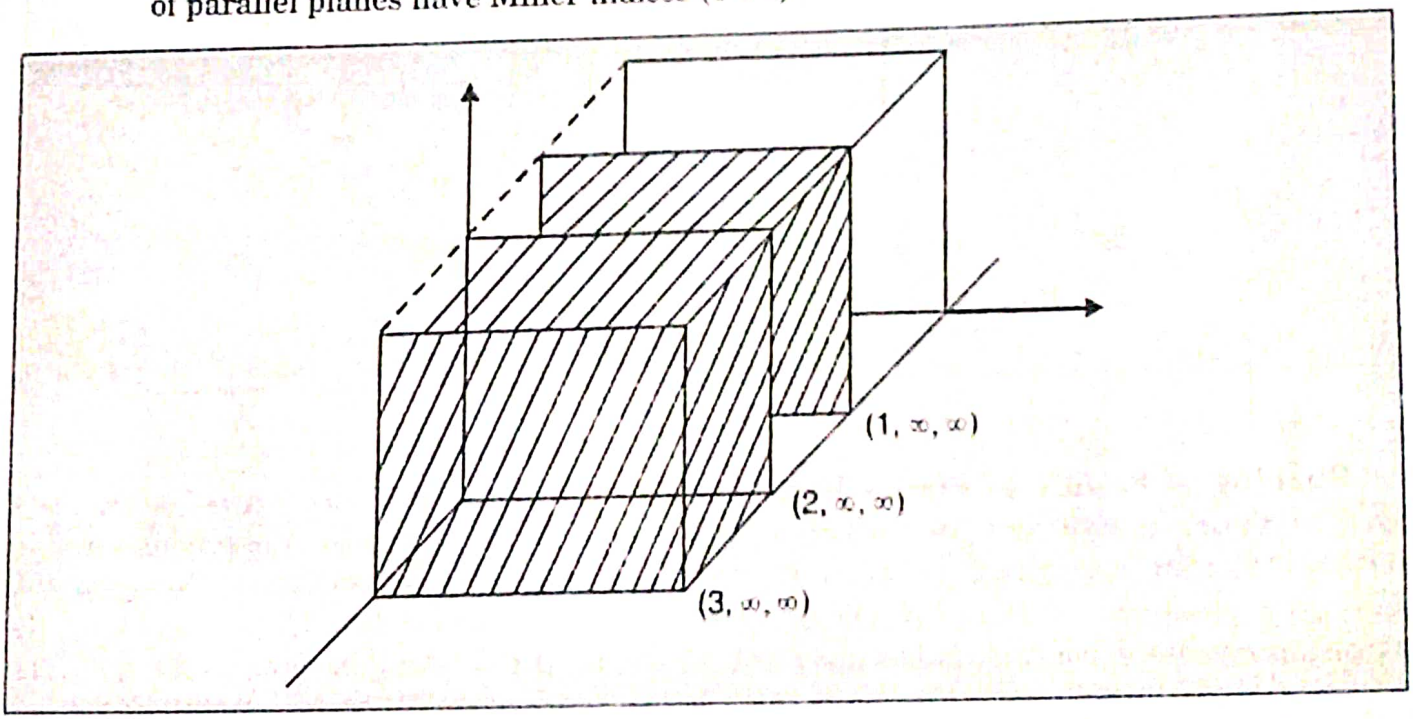


Fig. 1.30.

(ii) The intercept of the set of parallel planes shown in Fig. 1.31 are $(\infty, \frac{1}{2}, \infty)$, $(\infty, \frac{2}{2}, \infty)$ and $(\infty, \frac{3}{2}, \infty)$. Hence all the planes have Miller indices (0 2 0)

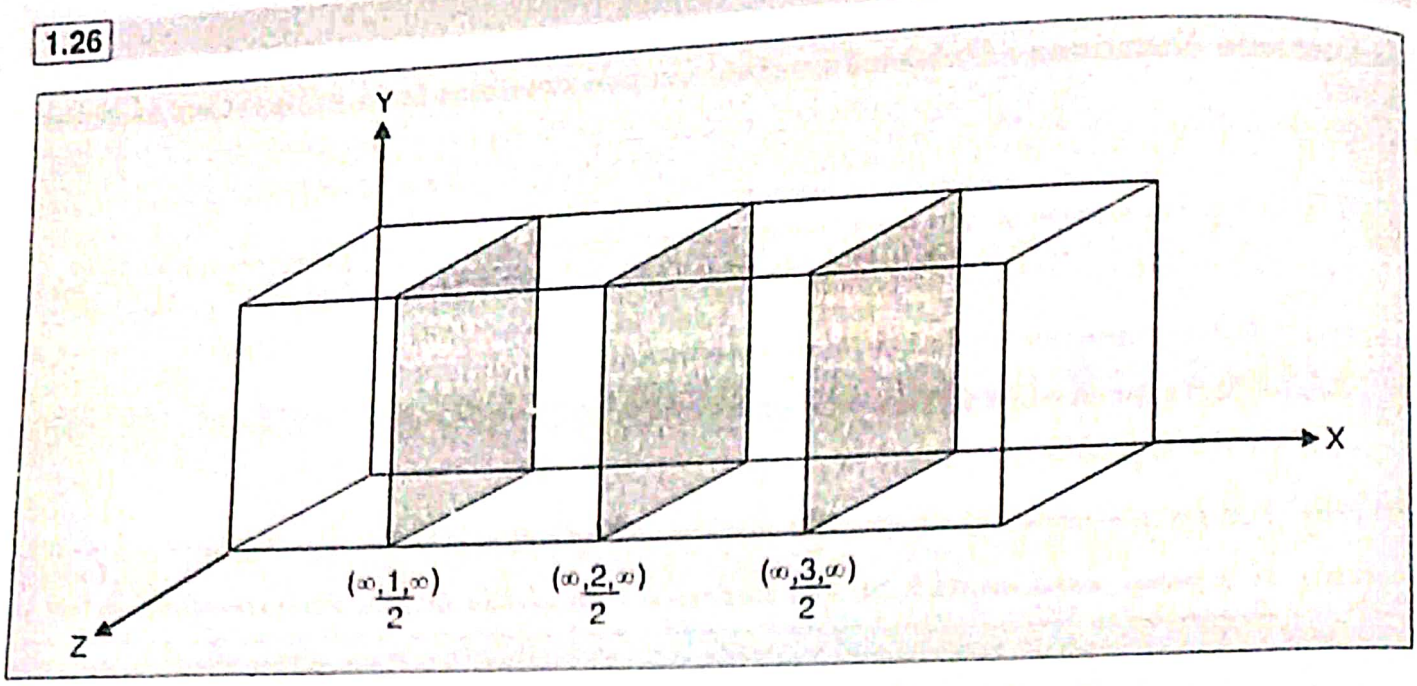


Fig. 1.31.

(iii) The Miller indices of the plane shown in Fig. 1.32 are $(\bar{1}\ 0\ 0)$

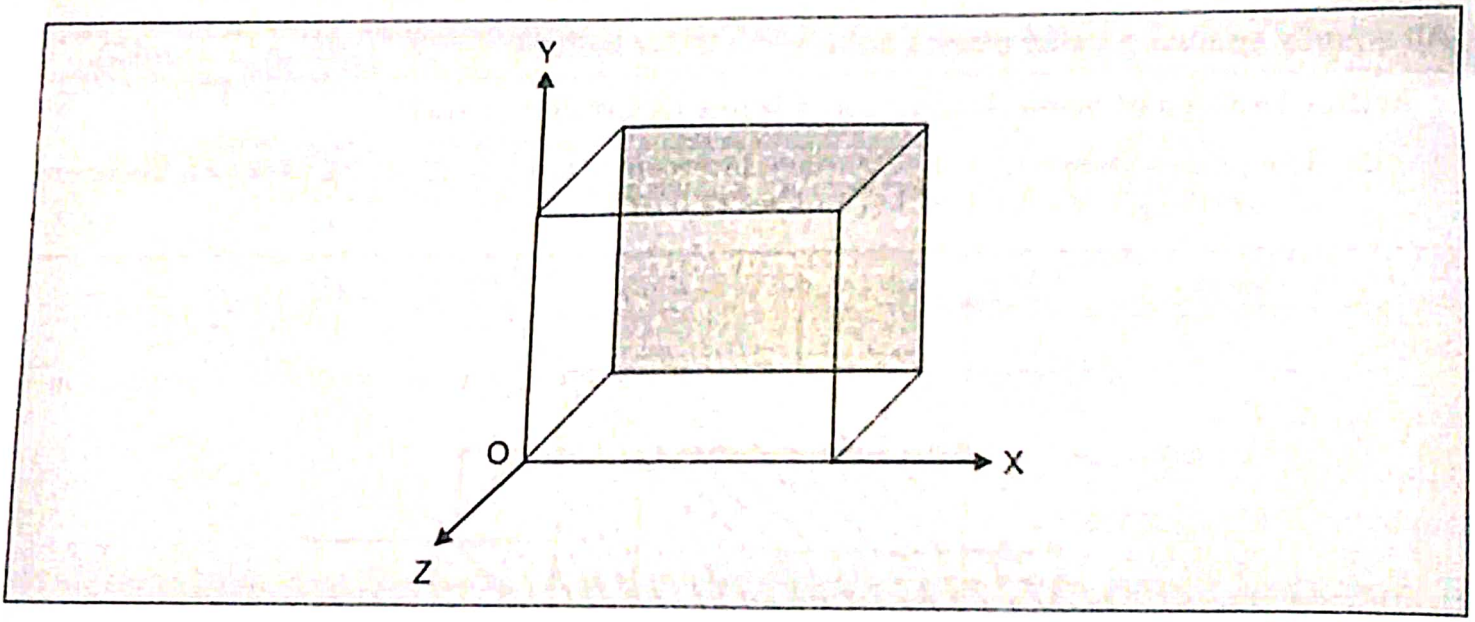


Fig. 1.32.

Spacing of Family of Planes Represented by (h k l) : If we have a set or family of parallel planes in a given crystal which is formed by a lattice and basis, these planes have a certain constant separation between them. Let the spacing or separation between two successive planes be "*d*". Let OX, OY and OZ be mutually perpendicular lines and form the cartesian system of coordinates as shown in Fig. 1.33. If this plane is represented by Miller indices (*h k l*), then the coordinates of A, B and C will be $\left(\frac{a}{h}, 0, 0\right)$, $\left(0, \frac{b}{k}, 0\right)$ and $\left(0,\ 0,\ \frac{c}{l}\right)$ respectively. Draw ON perpendicular to the plane ABC. If a plane parallel to plane ABC is taken, it will pass through the origin O such that ON = d is the minimum distance between two adjacent planes of this family. ON makes some angles α, β and γ with the three coordinate axes. In ΔONA (Fig. 1.34), we have

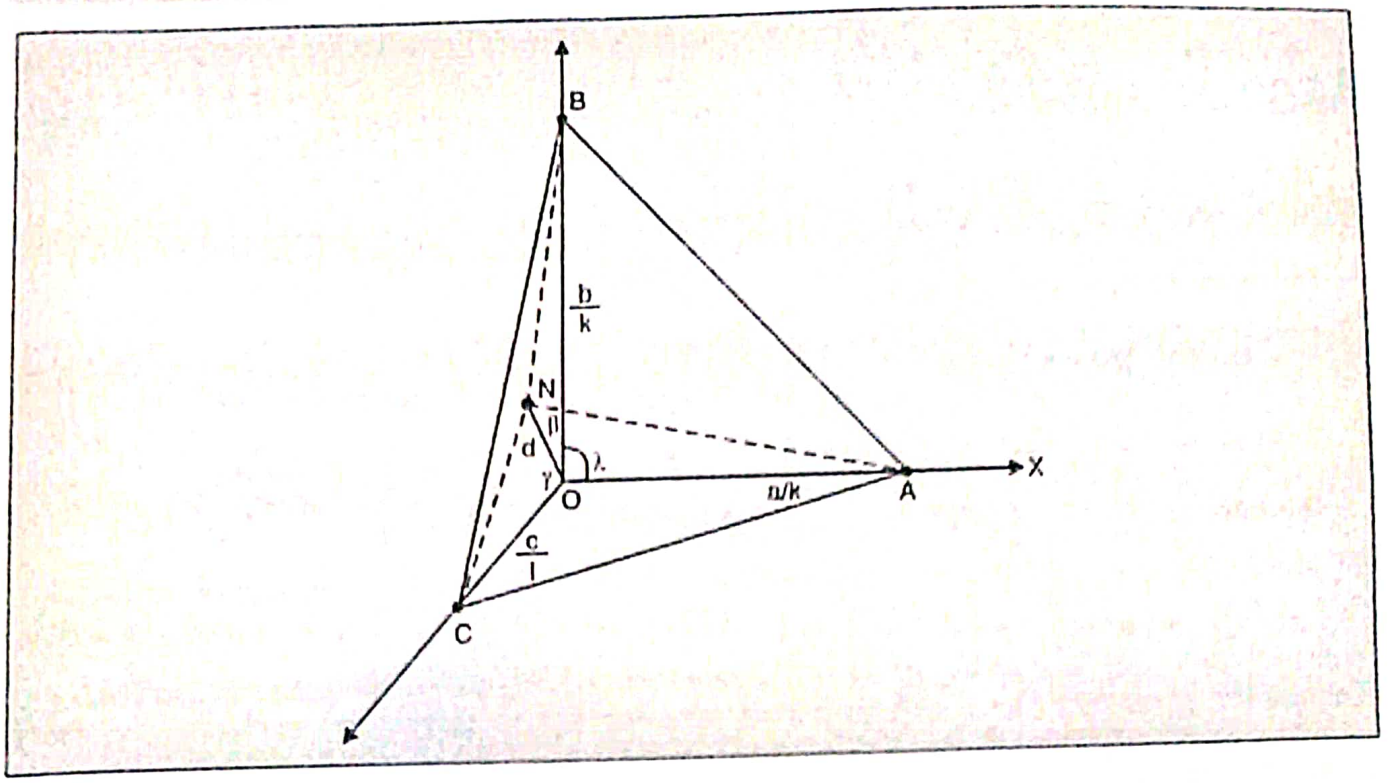


Fig. 1.33

$$\cos\alpha = \frac{ON}{OA}$$

Also $$\cos\beta = \frac{ON}{OB}$$

and $$\cos\gamma = \frac{ON}{OC}$$

or $$ON = OA\cos\alpha$$

or $$d = \left(\frac{a}{h}\right)\cos\alpha$$

Hence, $$\cos\alpha = d\left(\frac{h}{a}\right)$$

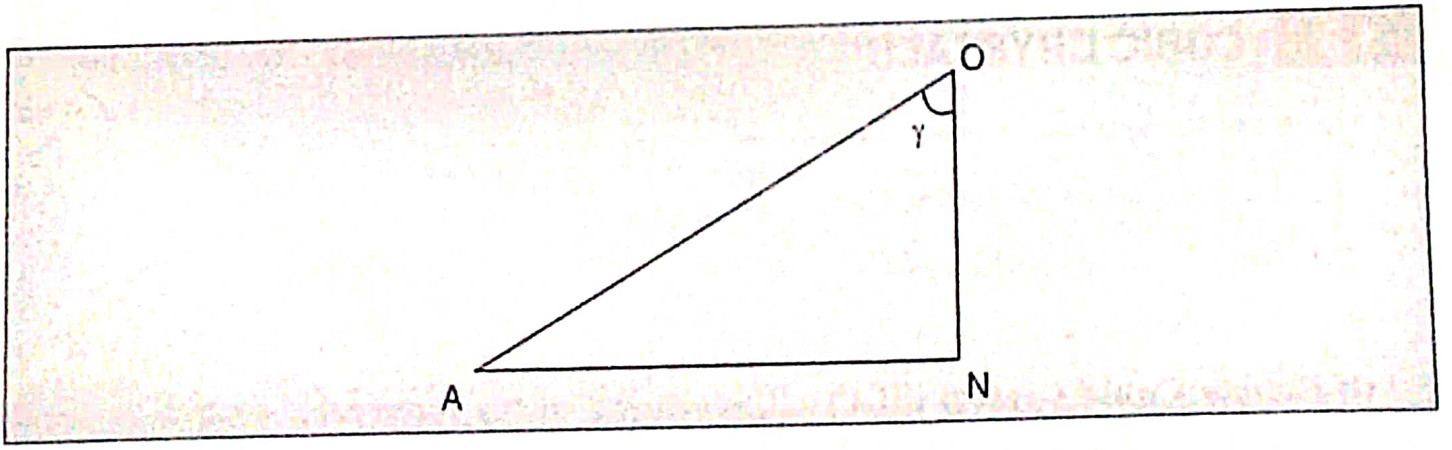


Fig. 1.34.

Similarly $\cos\beta = d\left(\frac{k}{b}\right)$

and $\cos\gamma = d\left(\frac{l}{c}\right)$

Since we know that

$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$

Substituting the values of $\cos\alpha$, $\cos\beta$ and $\cos\gamma$

We have

$$\left[d\left(\frac{h}{a}\right)\right]^2 + \left[d\left(\frac{k}{b}\right)\right]^2 + \left[d\left(\frac{l}{c}\right)\right]^2 = 1$$

$$\text{or } d^2\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right] = 1$$

$$\text{or } d^2 = \frac{1}{\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right]}$$

For a cubic system,

$a = b = c$, so that we have

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

The formula for inter planer spacing d shows that the greater are the plane indices the shorter is the distance between the planes.

1.8 CUBIC CRYSTALS

There are three types of cubic crystals

(i) Simple Cubic Crystal (SCC)

(ii) Body Centered Cubic (BCC)

(iii) Face Centered Cubic (FCC)

(i) Simple Cubic Crystal (SCC) : The simplest of the three cubic crystals is simple cubic as shown in Fig. 1.35. The lattice points are only at the corners of cube. This type of unit cell is primitive type. Hence there is only one atom at each corner of the cube.

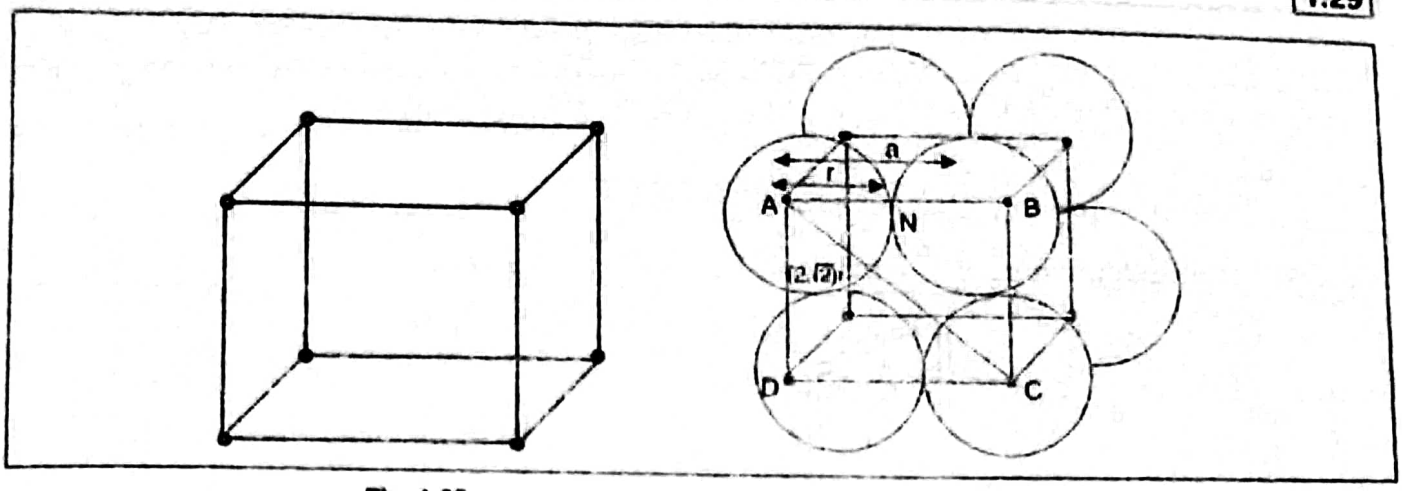


Fig. 1.35.

Fig. 1.36.

The three dimensional structure of SCC is drawn by placing the atoms touching with each other as shown in Fig. 1.36. Examples of SCC are CaCl, NH_4Cl etc.

(ii) Body Centered Cubic (BCC) : Here eight atoms are present at each corner and one atom is present at the centre of the cube as shown in Fig. 1.37. The three dimensional structure of BCC is shown in Fig. 1.38. The examples of BCC are Na, Rb, Ta, W etc.

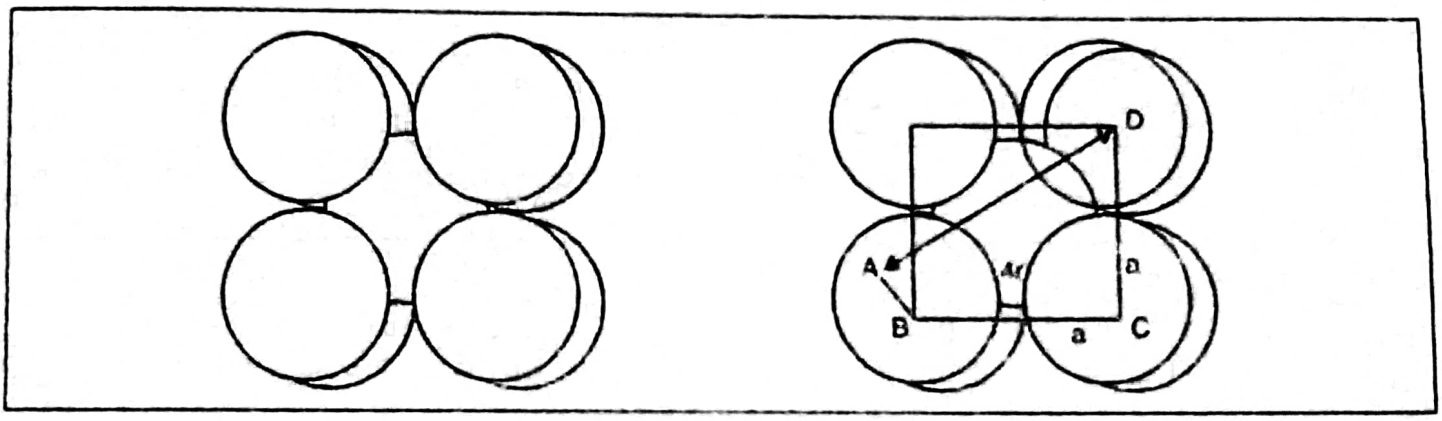


Fig. 1.37.

Fig. 1.38.

(iii) Face Centered Cubic (FCC) : There are eight atoms at the corners and six atoms are there at the six faces of the cube. As every face is shared by two cubes so half atom at each face belongs to one cube. The examples of FCC are Cu, Al, Pb, Ag etc. The unit cell of FCC is shown in Fig. 1.39.

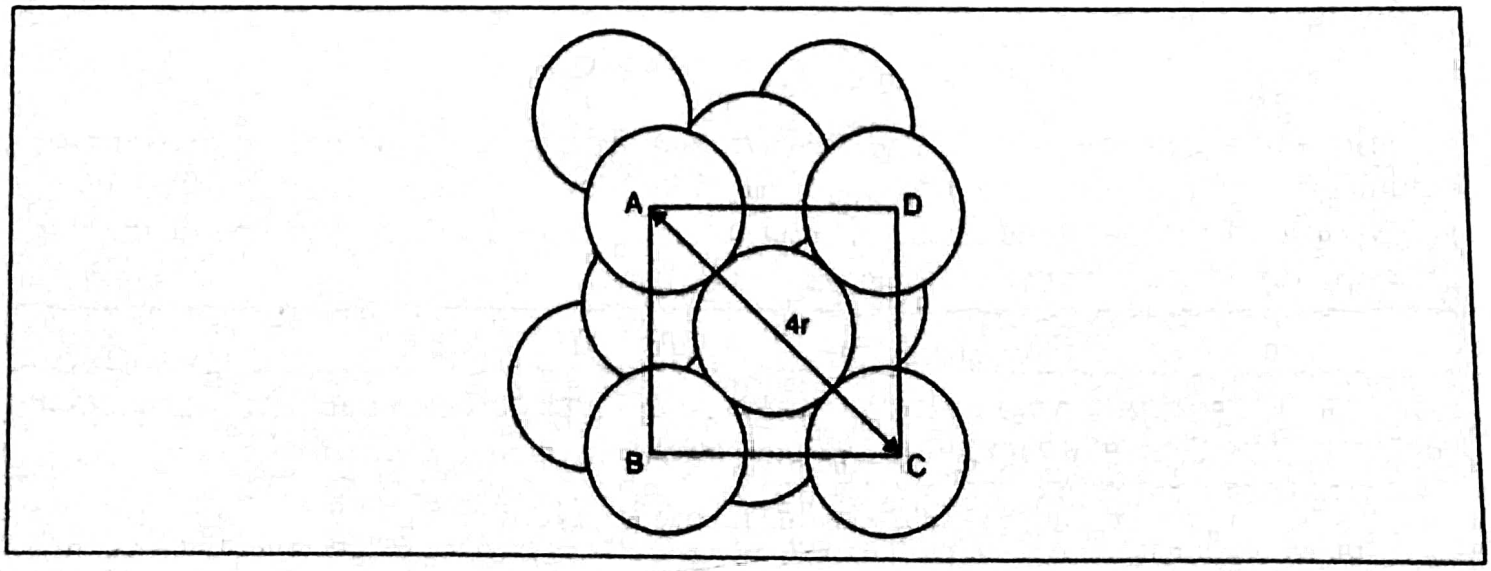


Fig. 1.39.

Point to Remember

SCC is a primitive cell whereas BCC and FCC are non-primitive cells.

1.9 CHARACTERISTICS OF A UNIT CELL

(i) Number of Atoms per Unit Cell (N) : If N_i is the number of interior atoms, N_f is the number of face centered atoms and N_c is the number of corner atoms then the total number of atoms per unit cell (N) are given by the relation.

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

Therefore, for SCC, we have

$$N = 0 + 0 + \frac{8}{8}$$

$$= 1$$

for BCC,

$$N = 1 + 0 + \frac{8}{8}$$

$$= 2$$

and for FCC

$$N = 0 + \frac{6}{2} + \frac{8}{8}$$

$$= 4$$

(ii) Volume of a Unit Cell : We know that for cubic crystals, $a = b = c$, therefore the volume of unit cell,

$$V = a \times b \times c$$

$$= a^3$$

(iii) Coordination Number : The coordination number is defined as the number of equidistant nearest neighbours that an atom has in the given structure. The physical significance of the coordination number is that it is a measure of closeness of packing of atoms in any given structure.

Point to Remember

For simplicity of writing we write "atoms" though these particles could be atoms or Ions or molecules, depending upon the system taken.

The coordination number for three cubic lattices can be determined as follows :

(a) SCC : If one corner atom is taken to be at the centre then it is found that there are six

nearest neighbours to this atom. Hence the coordination number for SCC is 6 as shown in Fig. 1.40.

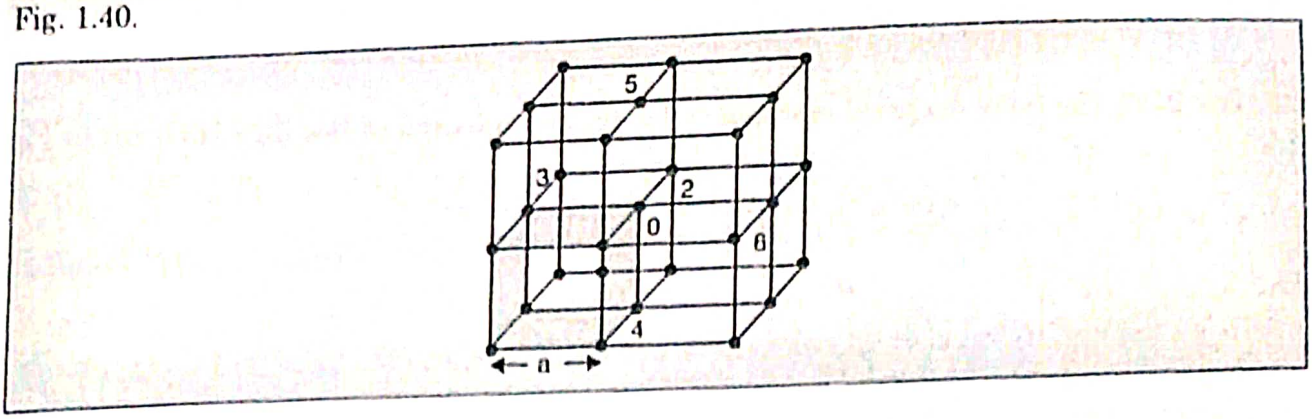


Fig. 1.40.

(b) BCC : There are eight atoms at the corners in BCC and there is one atom in the centre of the body of cube. Taking into the account, the central atom, we observe that there are eight nearest atoms. Therefore the coordination number for BCC structure is 8 as shown in Fig. 1.41.

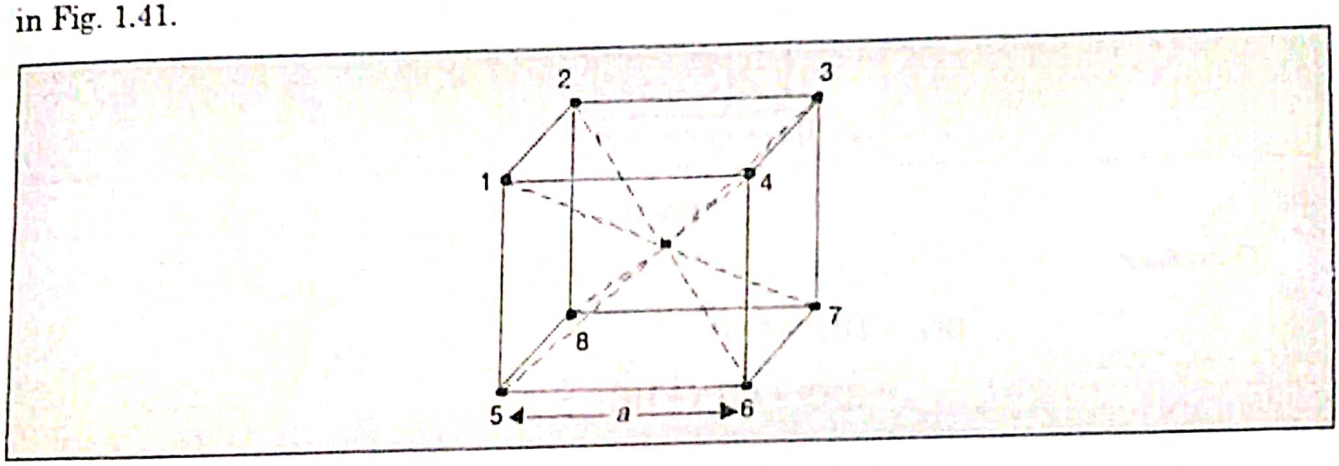


Fig. 1.41.

(c) FCC lattice : In FCC lattice, an atom at the face is surrounded by twelve atoms. Therefore the coordination number for FCC lattice is 12 as shown in Fig. 1.42.

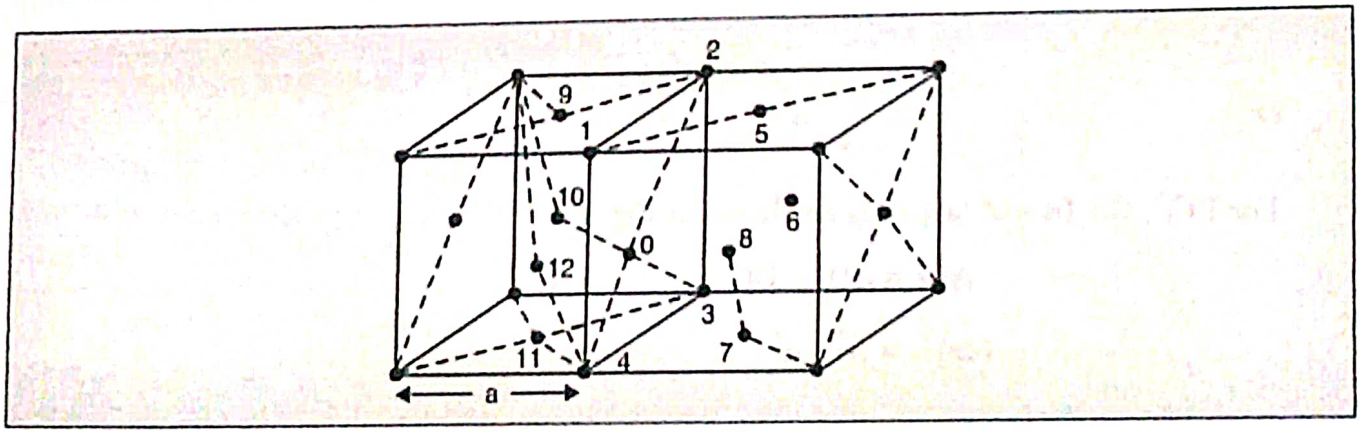


Fig. 1.42.

(iv) Atomic Radius : The size of the atoms allowed is controlled by the nature of the system. Thus the value of radius of atom is different for each of the SCC, Bcc and FCC systems. Atomic radius is actually half the distance between the nearest neighbours.

For SCC, the atomic radius r is given by

$$r = \frac{a}{2}$$

For BCC, the body diagonal is taken to be $4r$. The unit cell of Bcc type is shown in Fig. 1.43.

$$DH^2 = DC^2 + CH^2$$

$$= a^2 + a^2$$

$$= 2a^2$$

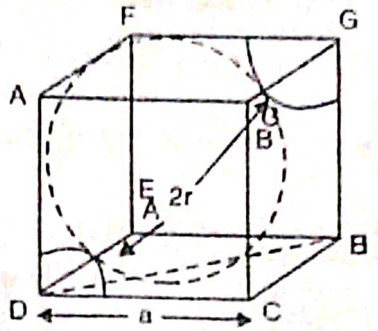


Fig. 1.43.

Therefore

$$DG^2 = DH^2 + HG^2$$

$$= (DC^2 + CH^2) + HG^2$$

$$= (a^2 + a^2) + a^2$$

$$(4r)^2 = 2a^2 + a^2$$

$$= 3a^2$$

or $$r = \frac{\sqrt{3}}{4} a$$

For FCC, the face of lattice is as shown in Fig. 1.44.

$$AC^2 = AD^2 + DC^2$$

$$(4r)^2 = a^2 + a^2$$

$$= 2a^2$$

or the radius $$r = \frac{\sqrt{2}}{4} a$$

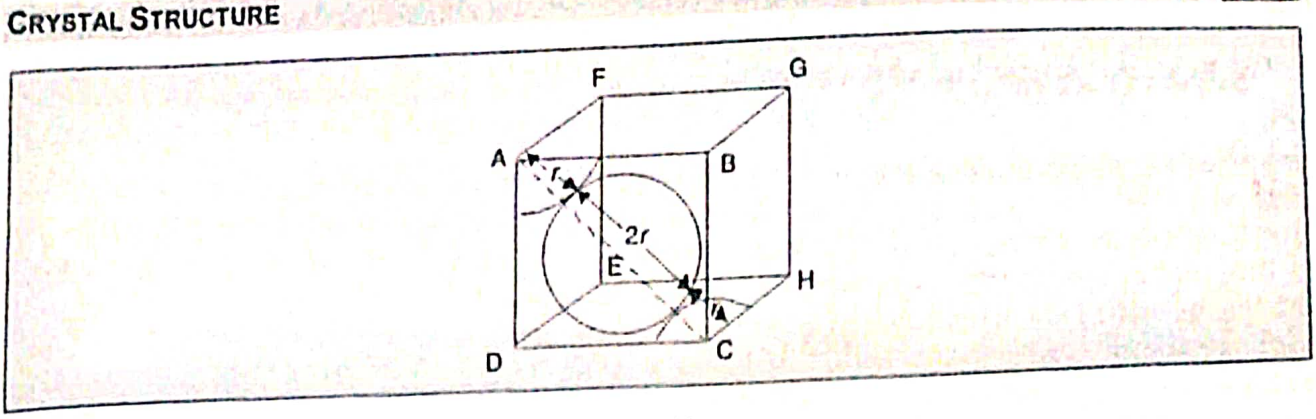


Fig. 1.44.

(v) Packing Fraction : We know that all the available volume is not fully filled up with atoms. In fact, there are empty spaces left out. These empty spaces differ from system to system.

Packing fraction is defined as the ratio of the volume occupied by all atoms in a unit cell to the total volume of the unit cell.

$$\text{Atomic packing fraction (P.F.)} = \frac{\text{Volume of all the atoms in a unit cell}}{\text{Volume of unit cell}}$$

$$= \frac{\text{Volume of one atom} \times \text{No. of atoms per unit cell}}{\text{Volume of unit cell}}$$

$$= \frac{\frac{4}{3}\pi r^3 \text{N}}{a^3}$$

$$= \frac{4\pi r^3 \text{N}}{3a^3}$$

For a SCC, number of atoms per unit cell, N = 1

radius of each cell $r = \frac{a}{2}$

$$\text{Hence packing fraction (P.F.)} = \frac{4\pi r^3 \text{N}}{3a^3}$$

$$= \frac{4\pi a^3 \times 1}{3a^3 \times 8}$$

$$= \frac{\pi}{6}$$

$$= 0.52$$

Thus, the space occupied by atoms in SCC is only 52% of the available space.

For a BCC structure, number of atoms per unit cell N = 2

radius of each cell, $r = \frac{\sqrt{3}\,a}{4}$

Hence packing fraction P.F.

$$= \frac{4\pi r^3 N}{3a^3}$$

$$= \frac{4\pi 3\sqrt{3}\,a^3 2}{3a^3 \times 64}$$

$$= \frac{\sqrt{3}\,\pi}{8} = 0.68$$

Thus, space occupied by atoms in BCC structure is only 68% of the available space.

(vi) Density of Unit Cell : Density of unit cell of a crystalline material is the ratio of mass of a unit cell to its volume. The mass of a single atom can be obtained by dividing the atomic mass A by Avogadro's number N_0

$\therefore$ Mass of a single atom $= \frac{A}{N_0}$

Mass of the unit cell $= N\left(\frac{A}{N_0}\right)$

where N is the number of atoms per unit cell.

Now density $\rho = \frac{\text{mass}}{\text{volume}}$

$$= \frac{N\left(\frac{A}{N_0}\right)}{\frac{4}{3}\pi r^3}$$

For SCC, BCC and FCC systems the value of N is 1, 2 and 4 respectively. The volume V a^3 for all the systems,

Hence, $\rho_{SCC} = \frac{1A}{N_0 a^3}$

$$\rho_{BCC} = \frac{2A}{N_0 a^3}$$

and $\rho_{FCC} = \frac{4A}{N_0 a^3}$

Thus $\rho_{SCC} < \rho_{BCC} < \rho_{FCC}$

Actually the size of unit cell or the radius r decreases as we go from SCC through BCC to FCC systems. Therefore the density increases with the increase in the value of N.

(vii) Polymorphism : If a crystal exists in more than one form, it observes the property of polymorphism. Thus the property of crystallizing in two or more forms is called polymorphism. Materials such as $CaCO_3$ which exist in two crystal forms are said to be dimorphous while materials like TiO_2 which exist in three forms are trimorphous. Iron (Fe) also shows polymorphism as it exists in BCC structural form below the curie temperature (*i.e.* 1042K) and in FCC structural form above the curie temperature. Similarly, cobalt exhibits the property of polymorphism as it shows FCC or hexagonal close packing structural form under different conditions.

1.10 HEXAGONAL CLOSE-PACKED STRUCTURE

The hexagonal close-packed structure unit cell has one atom at each corner and one atom at the centre of the hexagonal faces and has three more atoms within the body of the cell. Every atom is in contact with three atoms in the layer below its plane, six atoms in its plane and three atoms in the layer above. Therefore the coordination number for hexagonal close-packed structure becomes twelve.

As shown in Fig. 1.45, twelve atoms are located at the twelve corners and every corner is shared by six unit cells. Two central atoms at the base planes are shared half by each unit cell. Three full atoms lie in the unit cell. So, the effective number of atoms in a unit cell is six.

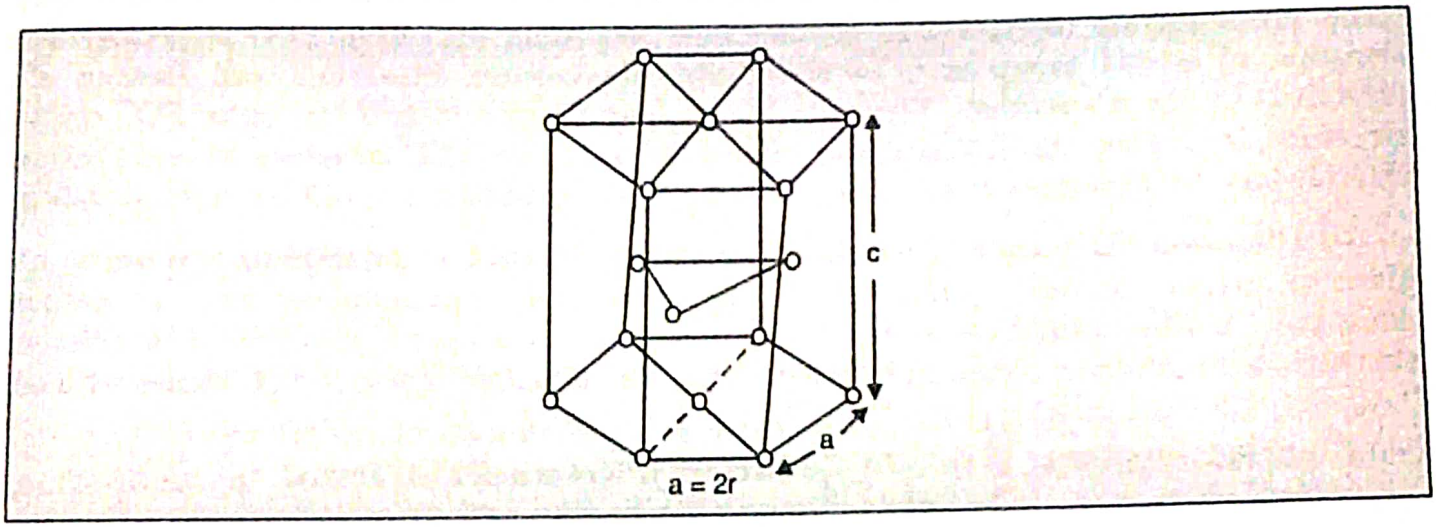


Fig. 1.45.

The calculations for the volume of unit cell can be made by taking the area of the base as

$$\text{area} = \frac{3\sqrt{3}\,a^2}{2}$$

Now volume of unit cell = area × cell's height c

$$= \frac{3\sqrt{3}\,a^2}{2}\,c$$

Since each corner is shared by six unit cells, so the volume of atoms in a unit cell

$$= 6 \times \frac{4}{3}\pi\lambda^3$$

$$= 8\pi \frac{a^3}{8} = \pi a^3$$

$$\text{Now, packing fraction} = \frac{\text{volume occupied by atoms}}{\text{volume of the cell}}$$

$$= \frac{\pi \; a^3}{\frac{3 \; \sqrt{3} \; a^2 \; c}{2}}$$

$$= \frac{2\pi}{3\sqrt{3}} \left(\frac{a}{c}\right)$$

$$= \frac{2\pi}{3\sqrt{3}} \sqrt{\frac{3}{8}} \qquad \left(\because \frac{c}{a} = \sqrt{\frac{8}{3}}\right)$$

$$= 0.74$$

1.11 SOME CRYSTAL STRUCTURES

Majority of metals are crystalline in nature. Simple cubic structure is very rare in metals. Some alkali metals like lithium, sodium and potassium etc. have BCC structure. The elements of second group such as Beryllium, Magnesium, Strontium and Barium etc. crystallise in *h c p* structure. Elements like copper, silver and gold etc. show FCC crystal structure. In non-metals, diamond and sodium chloride have FCC structure whereas cesium chloride has cubic crystal lattice. All noble gases crystallizes in either FCC or *h c p* structure.

(i) Diamond Structure : Elemental semiconductors such as germanium and silicon has diamond lattice as basic lattice structure. Compound semiconductor such as gallium phosphide, indium tungstate and indium phosphide have atoms arranged in a diamond structure with different atoms on alternate sites. The diamond lattice is FCC lattice with one additional lattice point at $\frac{\vec{a}}{4} + \frac{\vec{b}}{4} + \frac{\vec{c}}{4}$ distance from each of FCC atoms.

The diamond is the best example of three dimensional lattice with a basis as shown in Fig. 1.46.

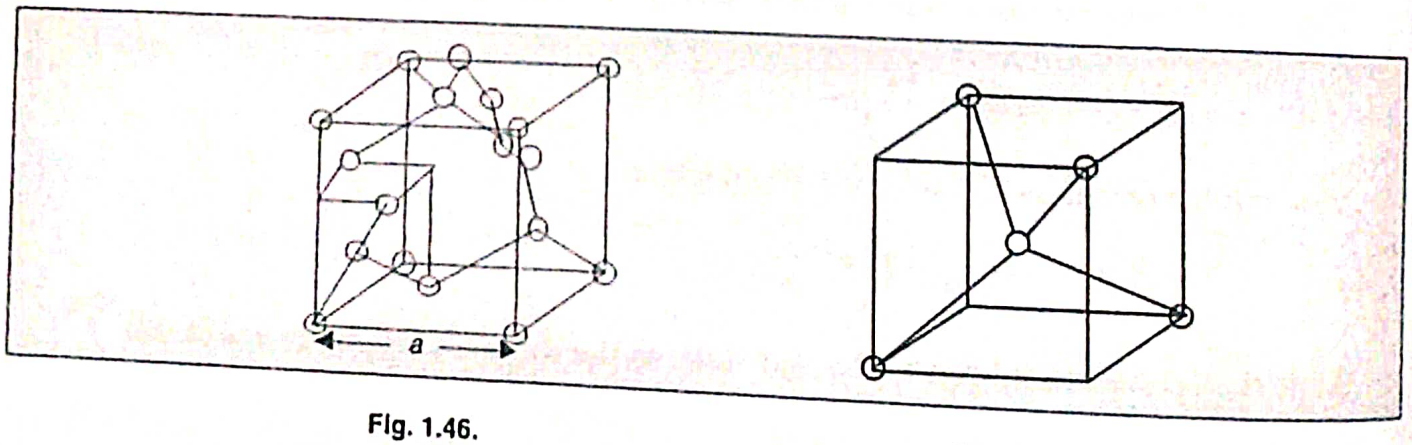


Fig. 1.46.

Fig. 1.47.

The diamond lattice in three dimensions can be obtained by inserting one FCC lattice into another FCC lattice displaced along the space diagonal by one fourth of its length. Fig. 1.47 shows a tetrahedron which depicts that in the diamond lattice every atom is surrounded by four nearest neighbours in the apexes of the tetrahedron whose edge is $a/2$.

There are eight atoms per unit cell. Four atoms are present in bulk per unit cell. Three atoms per unit cell are from faces and one atom per unit cell is from corners. The diagonal of the body of the cell is $8r$. The edge length of the unit cell shown in Fig. 1.46 is a.

$$(8r)^2 = 3a^2$$

$$a^2 = \frac{(8r)^2}{3}$$

or

$$a = \frac{8}{\sqrt{3}} r$$

Volume occupied by atoms in the unit cell $v = 8 \times \frac{4}{3}\pi\lambda^3$ and volume of unit cell $V = a^3 = \frac{512}{3\sqrt{3}} r^3$

$$\text{Thus the packing fraction} = \frac{\text{Volume occupied by atoms in unit cell}}{\text{Volume of unit cell}}$$

$$= \frac{\sqrt{3}}{16}\pi$$

$$= 0.34$$

This shows that the lattice of the diamond atom is relatively empty. The maximum value of the available volume which may be filled by hard spheres is only 0.34.

(ii) Sodium Chloride Structure : The structure of rock salt *i.e.* sodium chloride (NaCl) is shown in Fig. 1.48. The Bravais lattice for NaCl is FCC. The basis contains one sodium atom and one chlorine atom. In each unit cell four units (may be atoms or molecules) of NaCl are there.

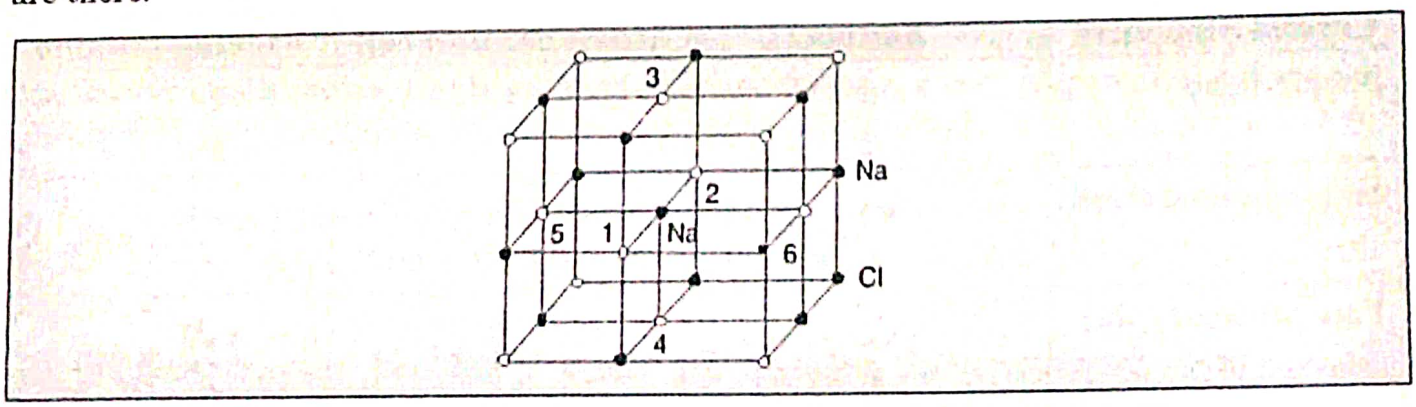


Fig. 1.48.

Fig. 1.48 shows that each atom of Na has six nearest Cl atoms. For example Na atom in

the centre is surrounded by six chlorine atoms labelled in the figure. Thus the coordination number is six.

To understand sodium chloride crystal, consider two FCC lattices one comprising of Na^+ ions and second of Cl^- ions. Place the two lattices coinciding with each other. Now displace one lattice with respect to second along either of axis by $\frac{a}{2}$. It will result in NaCl lattice.

LiH, KCl, PbS and AgBr are some other crystals having NaCl arrangement.

(iii) Cesium Chloride Structure [CsCl]. The structure of CsCl is shown in Fig. 1.49 which shows that the space lattice of cesium chloride is simple cubic [SCC]. The structure results from the combination of two simple cubic sub lattices, one of cesium and other of chlorine atom.

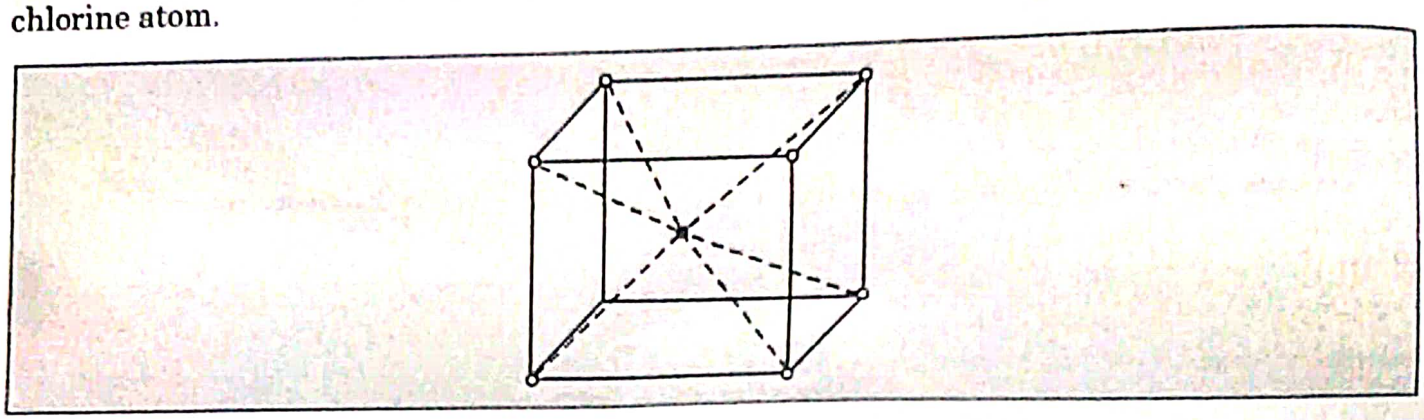


Fig. 1.49.

The basis has one cesium atom and one chlorine atom. The position of cesium is at (0, 0, 0) and that of chlorine atom is at $\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$ of the simple cubic space lattice. The Bravais lattice is BCC. Each cesium atom has eight chlorine atoms in the surroundings. To understand CsCl crystal, take two SC lattices, one comprising of cesium atoms and other of chlorine atoms. Place the two lattices coinciding with each other. When one lattice is displaced with respect to second along the diagonal by an amount equal to one half of the diagonal, then CsCl lattice results.

NH_4Cl, BeCu, TlI, TlBr and CuPd are some of the other crystals or compounds having the crystal structure like CsCl.

Crystal Structure	Radius	Atoms per unit cell	Packing fraction
Simple cubic	$\frac{a}{2}$	1	$\frac{\pi}{6} = 52\%$
Body centered cubic	$\frac{\sqrt{3}}{4}a$	2	$\frac{\pi\sqrt{3}}{8} = 68\%$
Face centered cubic	$\frac{\sqrt{2}}{4}a$	4	$\frac{\pi\sqrt{2}}{6} = 74\%$
Diamond	$\frac{\sqrt{3}\,a}{8}$	8	$\frac{\pi\sqrt{3}}{16} = 34\%$

1.12 RECIPROCAL LATTICE

Many properties of crystalline substances are different in different directions. W.H. Miller explained the concept of Miller indices to represent the planes and directions of a crystal. In real practice there are many set of planes with different orientations and spacings and it becomes difficult to visualise the slopes of the planes. Since all parallel planes have a common normal and similar indices, so the Miller indices of a plane can not be uniquely defined. Therefore to understand many crystallographic problems we consider the normal to be a set of planes rather than the planes themselves. The orientation of plane is understood by the direction of normal. To understand this we introduce the concept of reciprocal lattice.

So far in this chapter we have studied about directions, axis, unit vectors for crystals in real space where the quantities have the dimensions of length L. Now we will introduce reciprocal space where the crystal structure will be represented within a different frame work. In this space the dimensions of quantities are L^{-1}. This will help us to relate the crystal structure more easily to the waves of electrons travelling through it, as they are presented in the same framework.

Paul Peter Ewald (1888-1985), a German physicist and a crystallographer was the first to explain the concept of reciprocal space. Reciprocal space may be compared directly with the wave vector of an excitation of a photon, a lattice vibration or a moving electron. Multiplication of each coordinate with $\hbar$ converts reciprocal space into momentum space.

We know that any physical quantity which varies with time can be expressed as a sum of Fourier component in the frequency domain. Similarly, the spatial properties of a crystal can be described as the sum of components in Fourier space. Reciprocal lattice is also called K-space, Fourier space or momentum space.

Definition of Reciprocal Lattice : The reciprocal lattice in Fourier space is an infinite periodic three-dimensional array of points whose spacings are inversely proportional to the distances between planes in the direct lattice.

The need for devising the concept of the reciprocal lattice was to tabulate the two important properties of the crystal plane :

(i) Slopes of the planes

and (ii) inter planer spacings

Time-Crystals : Time crystals are systems where the role of space in ordinary crystalline crystals is replaced by time. As in ordinary crystals, a very large number of atoms, in principle an infinite number, display periodicity in space, similarly in time crystals they exibit periodicity in time. The importance of time crystals lies in the replacement of space by time. This idea was given by Frank Wilczek , a Nobel prize winner in 1975. The theoretical basis for the existence of time crystals was established in 2015 by Indian Physics Prof. Shivaji Sondhi.

In ordinary crystals, like NaCl, atoms are arranged in a repeating pattern and interactions between neighbour atoms keep the system rigid. A time crystal shows the same kind of rigid pattern as in regular crystal, but instead of being arranged in space, the pattern repeats in time. This repetition in time is small like the Earth's seasons which appear like clock work once a year.

Construction of Reciprocal Lattice : The concept of normals is used in the construction of reciprocal lattices. Martin Julian Buerger (1903-1986) an American crystallographer in 1948 was the first to construct the reciprocal lattice in his theoretical paper "Crystallographic symmetry in Reciprocal Space".

A reciprocal lattice from a direct lattice can be constructed as in the following steps :

(i) Take any point as an origin in direct lattice.

(ii) From this origin, draw normal to every set of planes in the direct lattice.

(iii) Set the length of every normal drawn equal to the reciprocal of the interplaner spacing $\left(\frac{1}{d_{hkl}}\right)$ of the set of parallel planes ($h\ k\ l$) it represents.

(iv) Place a point at the end of each normal.

The assembly of these points represents a lattice array which is called as "reciprocal lattice". This represent a tabulation of (i) the normals to all the direct lattice planes and (ii) their interplaner spacings. The direction of each of the points preserves the orientation of the set of parallel planes it represents. The distance of each of the points from the origin tells the interplaner spacing of that set of parallel planes.

Graphical Construction of Reciprocal Lattice : To study the graphical construction of reciprocal lattice the unit cell is oriented in such a way that an arbitrary point 0 is chosen as origin. The unit cell of monoclinic crystal along its unit axis designated by $\vec{b}$, $\vec{a}$ and $\vec{c}$ and representing the cell edges is shown in Fig. 1.50. It shows four ($h\ k\ l$) planes *viz.*, (100), (101), (102) and (001). All those planes are parallel to b and hence their normal lies in the plane of the paper.

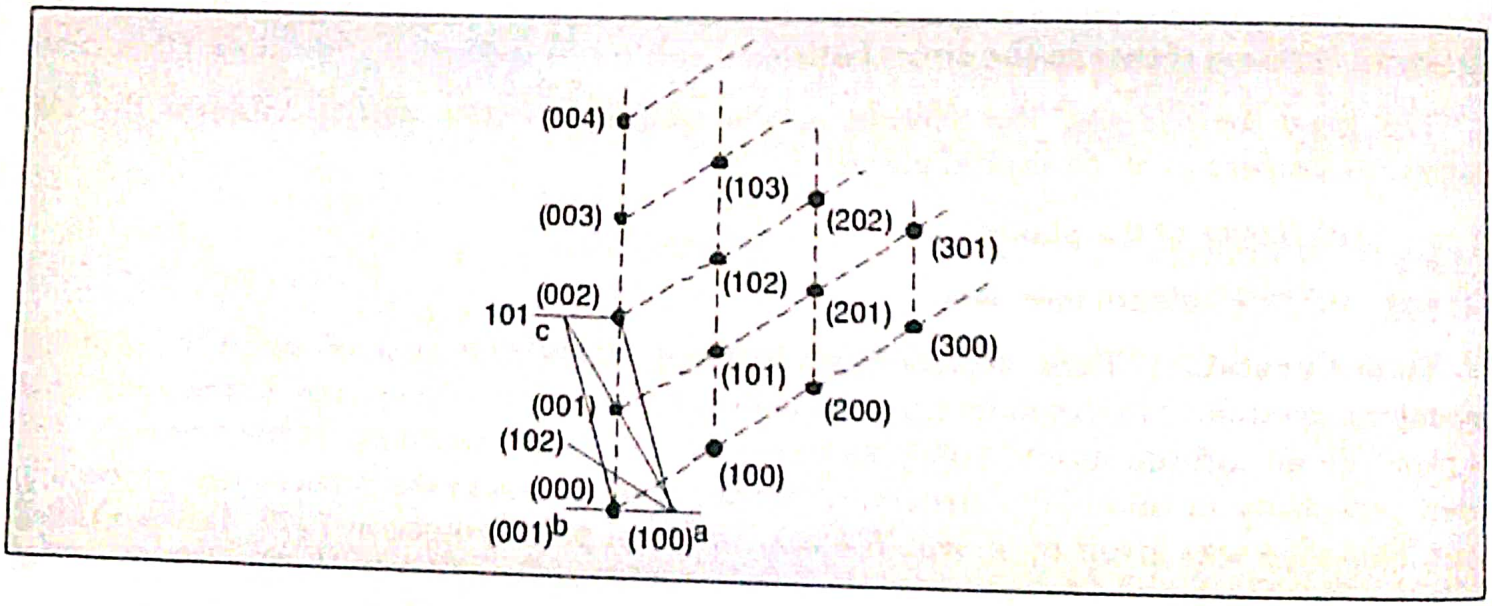


Fig. 1.50

In direct lattice the basis vectors are represented as $\vec{a}$, $\vec{b}$ and $\vec{c}$ whereas in the reciprocal lattice the basis vectors are represented as $\vec{A}$, $\vec{B}$ and $\vec{C}$. As per vector algebra, we have,

$\vec{a} \cdot \vec{A} = 1$, $\vec{a} \cdot \vec{B} = 1$ and $\vec{a} \cdot \vec{C} = 1$

$\vec{b} \cdot \vec{A} = 0$, $\vec{b} \cdot \vec{B} = 0$ and $\vec{c} \cdot \vec{B} = 0$

$\vec{a} \cdot \vec{C} = 1$, $\vec{b} \cdot \vec{C} = 0$ and $\vec{c} \cdot \vec{C} = 0$

Also $\vec{b} \cdot \vec{A} = 0$ and $\vec{c} \cdot \vec{A} = 0$

which implies, $\vec{A} \perp \vec{b}$ and $\vec{A} \perp \vec{c}$

Thus, $\vec{A}$ is perpendicular to $\vec{b}$ as well as $\vec{c}$.

Mathematically $\vec{A}$ is parallel to vector product of $\vec{b}$ and $\vec{c}$.

i.e. $$\vec{A} \propto (b \times c)$$

or $$\vec{A} = k(\vec{b} \times \vec{c})$$

Also, $$\vec{a} \cdot \vec{A} = 1$$

or $$\vec{a} \cdot k(\vec{b} \times \vec{c}) = 1$$

or $$k = \frac{1}{a.\left(\vec{b} \times \vec{c}\right)}$$

Hence,

$$\vec{A} = k(\vec{b} \times \vec{c}) = \frac{\vec{b} \times \vec{c}}{\vec{a}.\left(\vec{b} \times \vec{c}\right)}$$

Similarly,

$$\vec{B} = \frac{\vec{c} \times \vec{a}}{\vec{b}.\left(\vec{c} \times \vec{a}\right)}$$

and $$\vec{C} = \frac{\vec{a} \times \vec{b}}{\vec{c}.\left(\vec{a} \times \vec{b}\right)}$$

For simplicity, we multiply the right hand side by 2π, so that

$$\vec{A} = 2\pi \frac{\vec{b} \times \vec{c}}{\vec{a} \cdot \left(\vec{b} \times \vec{c} \right)}$$

$$\vec{B} = 2\pi \frac{\vec{c} \times \vec{a}}{\vec{b} \cdot \left(\vec{c} \times \vec{a} \right)}$$

and

$$\vec{C} = 2\pi \frac{\vec{a} \times \vec{b}}{\vec{c} \cdot \left(\vec{a} \times \vec{b} \right)}$$

$\vec{A}$, $\vec{B}$ and $\vec{C}$ are also called reciprocal lattice primitive vectors

Point to Remember

$\vec{A}$ is normal to $\vec{b}$ and $\vec{c}$

$\vec{B}$ is normal to $\vec{c}$ and $\vec{a}$

$\vec{C}$ is normal to $\vec{a}$ and $\vec{b}$

A point in the direct lattice is represented by translational vector $\vec{T}$ as

$$\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$$

where n_1, n_2 and n_3 are integers

Similarly, the reciprocal lattice vectors can be represented

$$\vec{G} = h\vec{A} + k\vec{B} + l\vec{C}$$

where $\vec{G}$ is called a reciprocal lattice vector, $\vec{A}$, $\vec{B}$ and $\vec{C}$ are primitive translation vectors

and h, k and $\vec{l}$ are integers.

A point (h, k, l) in the reciprocal lattice space corresponds to the set of parallel planes having the Miller indices (h, k, l)

Thus, every crystal structure has two lattices associated with it.

(i) crystal lattice

and (ii) reciprocal lattice

When we rotate a crystal, we rotate both the crystal lattice and the reciprocal lattice.

Point to Remember

The crystal lattice is a lattice in real or ordinary space whereas the reciprocal lattice is a lattice in the associated reciprocal space.

The points labelling the lattice planes $\vec{G}$ are called reciprocal lattice points and are defined by the relation

$$\vec{G} \cdot \vec{T} = 2\pi \times \text{integer}$$

or $$e^{i\vec{G}\cdot\vec{T}} = 1$$

where T is crystal translation vector.

Properties of Reciprocal Lattice : Reciprocal lattice is an invariant geometrical object whose properties are fundamental in the theory of solids. The elementary geometrical properties are as follows :

(i) The reciprocal lattice is a lattice in K-space or Fourier space. Direct lattice is a lattice in ordinary space.

(ii) The primitive vectors in reciprocal space have dimensions of (length)$^{-1}$. The primitive vectors of the direct lattice have the dimensions of length.

(iii) The reciprocal of the reciprocal lattice is the direct lattice.

(iv) The volume of a unit cell of the reciprocal lattice is inversely proportional to the volume of the unit cell of the direct lattice.

(v) Each point in a reciprocal lattice represents a set of parallel planes of the crystal lattice.

(vi) Each vector of the reciprocal lattice is normal to a set of lattice planes of the direct lattice.

(vii) If the component of reciprocal lattice vector $\vec{G}$ have no common factor then $|\ G\ |$ is inversely proportional to the spacing of the lattice planes normal to $\vec{G}$.

(viii) When we rotate a crystal, both direct lattice and reciprocal lattice rotate.

(ix) The unit cell of the reciprocal lattice need not be a parallelopiped. Actually, we do deal with the Wigner-Seitz cell of the reciprocal lattice. This is known as Brillouin Zone in K-space.

Geometrical Significance of Reciprocal Lattice : Consider a primitive cell of oblique lattice having $\vec{a}$, $\vec{b}$ and $\vec{c}$ as the primitive vectors of the lattice as shown in Fig. 1.51. The volume of the primitive cell formed by three crystal lattice vectors in the direct space is given by

$$V = (\vec{a} \times \vec{b}) \cdot \vec{c}$$

= Area of parallelogram PQRS × perpendicular distance between the faces PQRS and TUVW

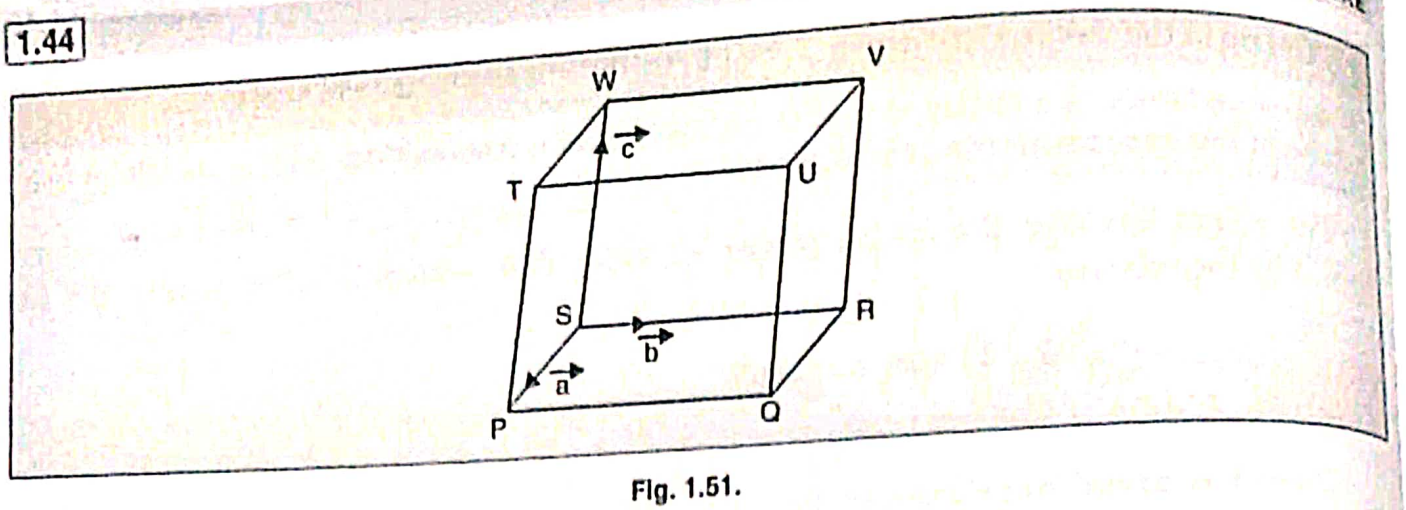


Fig. 1.51.

Now we know that the area of parallelogram PQRS is given by vector product of $\vec{a}$ and $\vec{b}$.

i.e. $$\text{Area} = \vec{a} \times \vec{b}$$

$$\frac{1}{d_{001}} = \left| \frac{\vec{a} \times \vec{b}}{\left(\vec{a} \times \vec{b}\right) \times \vec{c}} \right|$$

We also know that

$$\vec{C} = 2\pi \frac{\vec{a} \times \vec{b}}{\vec{c} \cdot \left(\vec{a} \times \vec{b}\right)}$$

$$= \frac{2\pi}{d_{001}} \left(\hat{a} \times \hat{b}\right)$$

Thus the physical significance of $\vec{C}$ is the vector whose magnitude is directly proportional to the reciprocal of inter planer separation between the planes having Miller indices (001) and the direction is always perpendicular to the plane (001) as shown in Fig. 1.52.

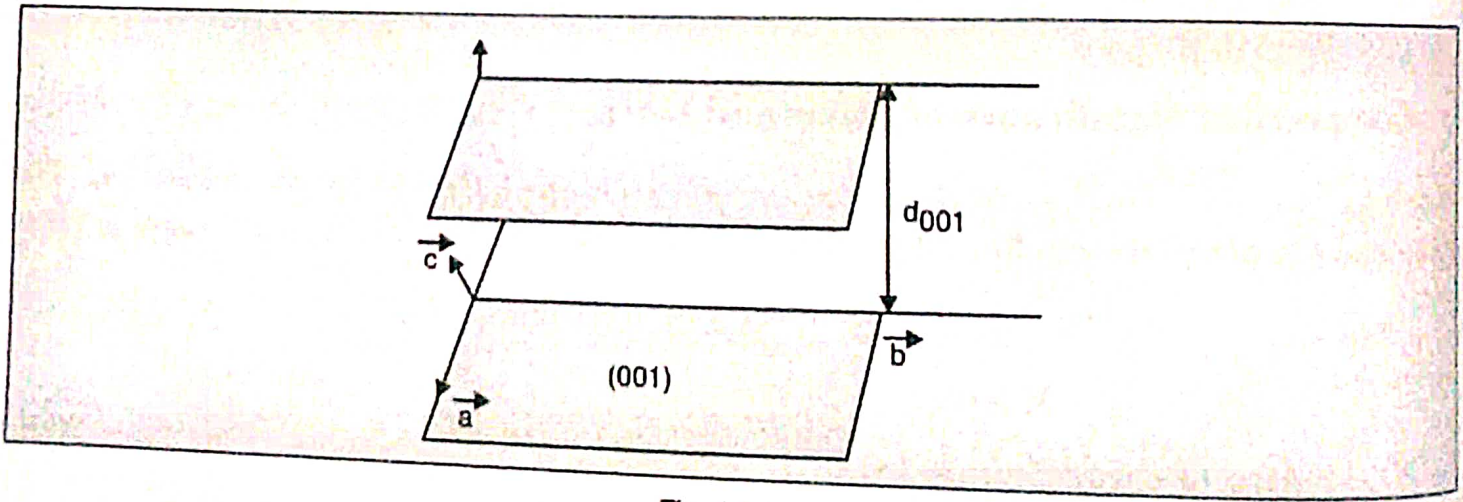


Fig. 1.52.

The tip of the vector $\vec{C}$ represents the plane (001) in the reciprocal space.

The physical significance of reciprocal lattice vector $\vec{B}$ is that it is that vector whose magnitude is directly proportional to the reciprocal of inter planer separation between the planes having Miller indices (010) and has direction perpendicular to the plane (010) as shown in Fig. 1.53.

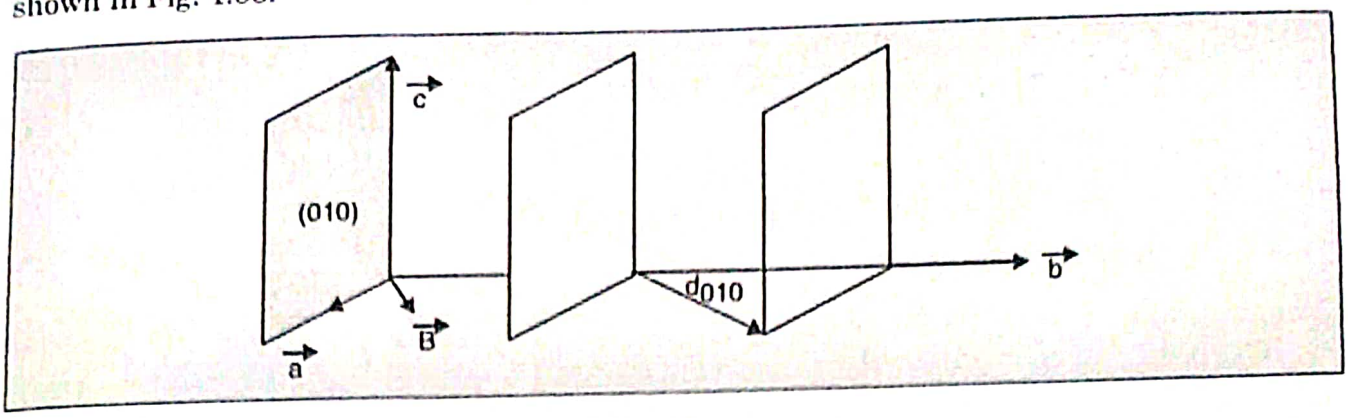


Fig. 1.53.

The tip of vector $\vec{B}$ represents the plane (010) in reciprocal lattice.

The physical significance of reciprocal lattice vector $\vec{A}$ is the vector whose magnitude is directly proportional to the reciprocal of inter planer separation between the planes having Miller indices and the direction is perpendicular to the plane (100) as shown in Fig. 1.54.

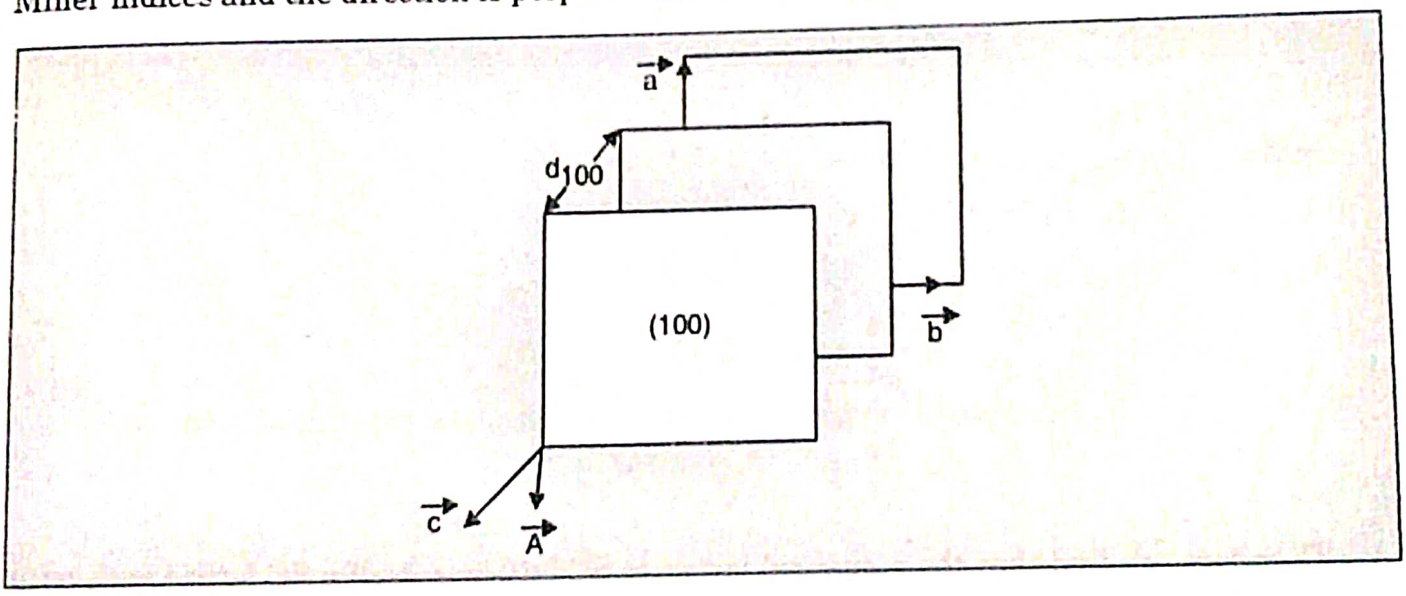


Fig. 1.54.

The tip of reciprocal lattice vector $\vec{A}$ represents the set of plane having Miller indices (100) in reciprocal lattice.

Reciprocal lattice to Simple Cubic : The primitive translation vectors of a simple cubic lattice are

$$\vec{a} = a\hat{i},\ \vec{b} = b\hat{j} \text{ and } \vec{c} = c\hat{k}$$

Here $a = b = c$ for simple cubic, so the volume of the cell in the direct lattice is

$$V = a \cdot (\vec{b} \times \vec{c})$$

$$= a^3$$

The primitive translation vectors of the reciprocal lattice are

$$\vec{A} = 2\pi \frac{(\vec{b} \times \vec{c})}{a(b \times c)}$$

$$= \frac{2\pi}{a^3} (a\,\hat{j} \times a\,\hat{k})$$

$$= \frac{2\pi}{a^3}\,\hat{i}$$

and

$$\vec{B} = 2\pi \frac{(\vec{b} \times \vec{c})}{b(c \times a)}$$

$$= \frac{2\pi}{a^3} (a\,\hat{k} \times a\,\hat{i})$$

$$= \frac{2\pi}{a}\,\hat{j}$$

and

$$\vec{C} = 2\pi \frac{\vec{a} \times \vec{b}}{c\left(\vec{a} \times \vec{b}\right)}$$

$$= \frac{2\pi}{a^3} (a\,\hat{i} \times a\,\hat{j})$$

$$= \frac{2\pi}{a^3}\,\hat{k}$$

Therefore, we find that the reciprocal lattice to SC lattice is itself a SC lattice with lattice constant $\frac{2\pi}{a}$.

Reciprocal lattice to Body Centered Cubic : Let $\vec{a}$, $\vec{b}$ and $\vec{c}$ be primitive basis vectors of body centered cubic cell (Fig. 1.55).

$$\vec{a} = \frac{a}{2} (\hat{i} + \hat{j} - \hat{k})$$

$$\vec{b} = \frac{a}{2}(-\hat{i} + \hat{j} + \hat{k})$$

$$\vec{c} = \frac{a}{2}(\hat{i} - \hat{j} + \hat{k})$$

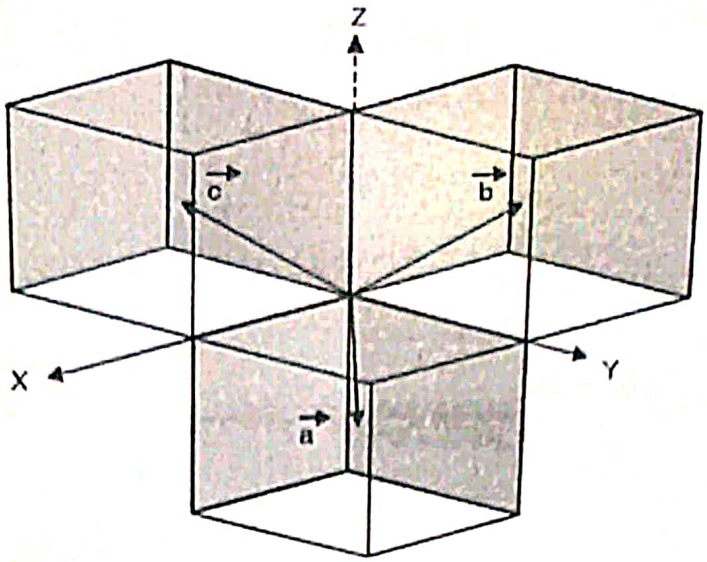


Fig. 1.55. Primitive basis vectors of BCC lattice

The volume of the cell in direct lattice is given by

$$V = \vec{a} \cdot (\vec{b} \times \vec{c})$$

$$= \frac{a}{2}(\hat{i} + \hat{j} - \hat{k}) \cdot \frac{a^2}{4} \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ -1 & 1 & 1 \\ 1 & -1 & +1 \end{vmatrix}$$

$$= \frac{a^3}{2}$$

Thus, the primitive translational vectors of the reciprocal lattice are

$$\vec{A} = 2\pi \frac{\vec{b} \times \vec{c}}{a.\left(\vec{b} \times \vec{c}\right)}$$

$$= 2\pi \left(\frac{2}{a^3}\right)\left(\frac{a^2}{4}\right) \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix}$$

$$= \frac{2\pi}{a}(\hat{i} + \hat{j})$$

and
$$\vec{B} = 2\pi \frac{\vec{c} \times \vec{a}}{\vec{b}\left(\vec{c} \times \vec{a}\right)}$$

$$= 2\pi \left(\frac{2}{a^3}\right)\left(\frac{a^2}{4}\right) \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix}$$

$$= \frac{2\pi}{a}(\hat{j} + \hat{k})$$

and
$$\vec{C} = 2\pi \frac{\vec{a} \times \vec{b}}{\vec{c}\left(\vec{a} \times \vec{b}\right)}$$

$$= 2\pi \left(\frac{2}{a^3}\right)\left(\frac{a^2}{4}\right) \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{vmatrix}$$

$$= \frac{2\pi}{a}(\hat{i} + \hat{k})$$

These primitive translational vectors are infact the primitive vectors of an FCC lattice. Hence an FCC lattice is the reciprocal lattice of the BCC lattice.

If h, k, l are integers, the $\vec{G}$ type reciprocal lattice vector is

$$\vec{G} = h\,\vec{A} + k\,\vec{B} + l\,\vec{C}$$

$$= \frac{2\pi}{a}[(h+l)\,\hat{i} + (h+k)\,\hat{j} + (k+l)\,\hat{k}]$$

The shortest $\vec{G}$ vectors are the following 12 vectors where all choices of the sign are independent

$$\frac{2\pi}{a}(\pm\,\hat{i} \pm \hat{j}),$$

$$\frac{2\pi}{a}(\pm\,\hat{j} \pm \hat{k}) \text{ and}$$

$$\frac{2\pi}{a}(\pm\,\hat{i} \pm \hat{k})$$

Reciprocal lattice to Face Centered Cubic : The primitive basis vectors of FCC are

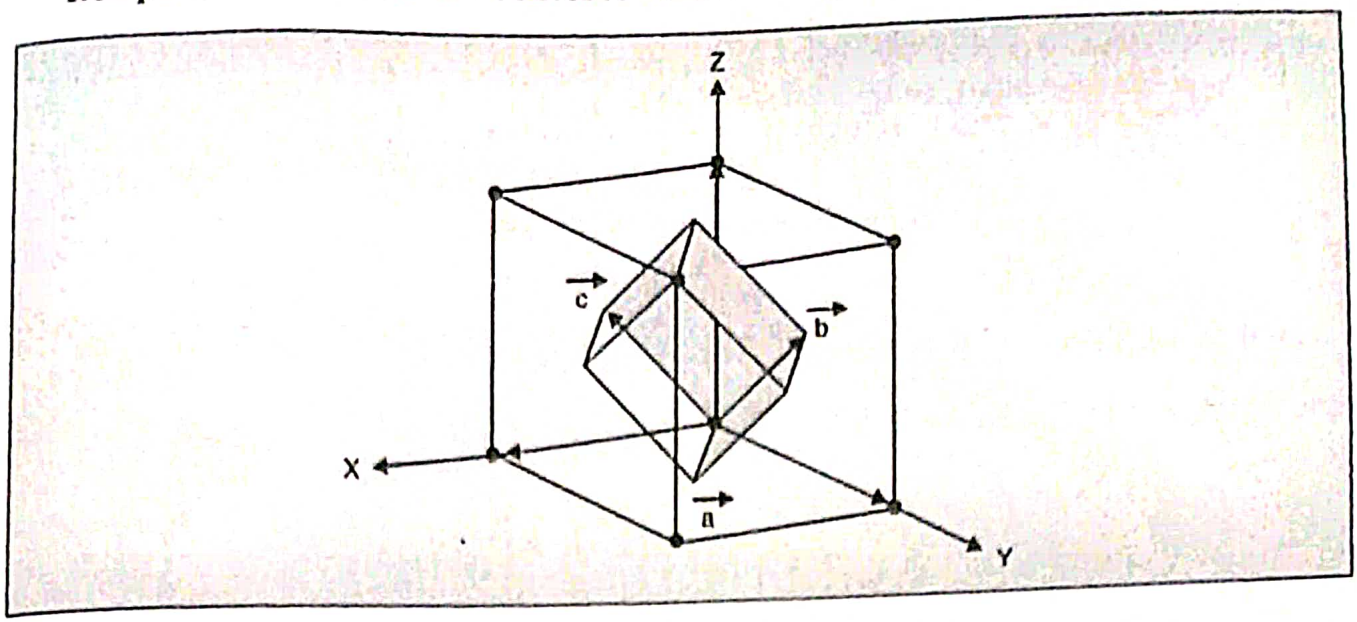


Fig. 1.56.

$$\vec{a} = \frac{a}{2}(\hat{i} + \hat{j})$$

$$\vec{b} = \frac{a}{2}(\hat{j} + \hat{k})$$

$$\vec{c} = \frac{a}{2}(\hat{i} + \hat{k})$$

The volume of the cell in direct lattice is

$$V = \vec{a} \cdot (\vec{b} \times \vec{c})$$

$$= \frac{a}{2}(\hat{i} + \hat{j})\left(\frac{a^2}{4}\right)\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix}$$

$$= \frac{a^3}{4}$$

The primitive translation vectors of the reciprocal lattice are

$$\vec{A} = 2\pi \frac{\left(\vec{b} \times \vec{c}\right)}{\vec{a} \cdot \left(\vec{b} \times \vec{c}\right)}$$

$$= 2\pi \left(\frac{4}{a^3}\right)\left(\frac{a^2}{4}\right)\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{vmatrix}$$

$$= \frac{2\pi}{a}(\hat{i} + \hat{j} - \hat{k})$$

and $$\vec{B} = 2\pi \frac{(\vec{c} \times \vec{a})}{\vec{a}.\left(\vec{b} \times \vec{c}\right)}$$

$$= (2\pi)\left(\frac{4}{a^3}\right)\left(\frac{a^2}{4}\right)\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix}$$

$$= \frac{2\pi}{a}(-\hat{i} + \hat{j} + \hat{k})$$

and $$\vec{C} = 2\pi \frac{\vec{a} \times \vec{b}}{\vec{c}.\left(\vec{a} \times \vec{b}\right)}$$

$$= 2\pi \left(\frac{4}{a^3}\right)\left(\frac{a^2}{4}\right)\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{vmatrix}$$

$$= \frac{2\pi}{a}(\hat{i} - \hat{j} + \hat{k})$$

These are the primitive translation vectors of a BCC lattice. Therefore, we conclude that the BCC lattice is the reciprocal lattice of the FCC lattice.

1.13 BRILLOUIN ZONE

A region bounded by the Wigner-Seitz plane in reciprocal lattice is a Brillouin Zone.

Linear lattice : Let us first discuss the formation of Brillouin Zones for a linear lattice. In one dimensional lattice the energy discontinuities occur when

$k = n\left(\frac{\pi}{a}\right)$ where n is a positive or negative integer, k is a wave vector and 'a' is the

lattice spacing. Kronig and Penny suggested the concept of periodically varying potential. They said that the energy spectrum consists of an infinite number of allowed energy bands separated by intervals in which there are no energy levels. These are called forbidden regions or bands. The boundaries of the allowed energy levels correspond to the values of $\cos k a = \pm 1$

or $$k a = n \pi$$

or $$k = \frac{n\pi}{a}$$

The above result $k = \pm \frac{n\pi}{a}$ can also be obtained from Bragg's reflection condition in reciprocal lattice to be discussed in next articles which states that if G is the translational vector in reciptocal lattice then,

$$\left(\vec{k} + \frac{\vec{G}}{2}\right) . \vec{G} = 0$$

or $$k = \pm \frac{G}{2}$$

$$= \pm \frac{n\pi}{a} \qquad \left(\because G = \pm \frac{2n\pi}{a}\right)$$

Hence, a line representing k values is divided by discontinuities in the energy. These discontinuities can be represented into segments of length $\pm \frac{\pi}{a}$. These line segments are referred as Brillouin Zones (Fig. 1.57). The first energy gap and the first reflection occurs at $k = \pm \frac{\pi}{a}$.

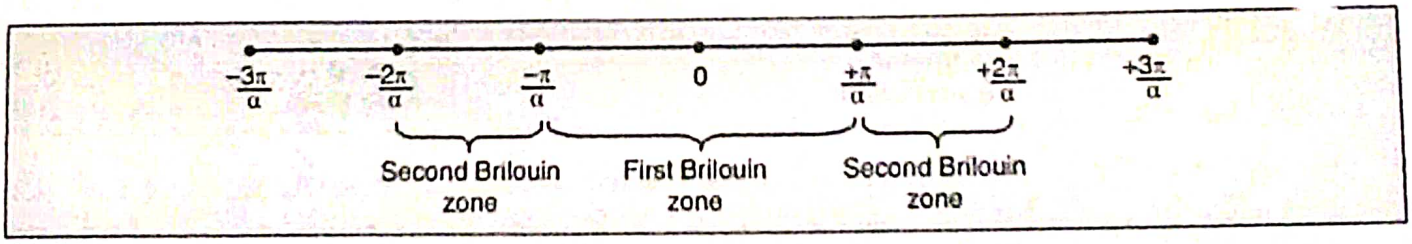


Fig 1.57

This reflection at $k = \pm \frac{\pi}{a}$ happens because the wave reflected from one atom in a linear lattice interferes constructively with the wave from nearest surrounding atom in the neighbourhood. The phase difference for the values of $k = + \frac{\pi}{a}$ and $k = - \frac{\pi}{a}$ between two reflected waves is $\frac{2\pi}{a}$. The region in K-space between $\frac{-\pi}{a}$ and $\frac{+\pi}{a}$ is called the first Brillouin Zone of the linear lattice.

Thus, the segment $\frac{-\pi}{a} \leq k \leq \frac{+\pi}{a}$ is known as the **first Brillouin Zone** of the lattice.

When the electrons have k-values between $\frac{\pi}{2}$ and $\frac{2\pi}{a}$ along the $\pm x$-direction, then the region is known as second Brillouin Zone. In this zone, the reflection and energy gap occurs at $k = \pm \frac{2\pi}{a}$. Similarly the formation of third, fourth etc. Brillouin Zones can be discussed.

When we plot a graph between the values of energy (E) in eV corresponding to the various values of $\vec{k}$, the graph is as shown in Fig. 1.58.

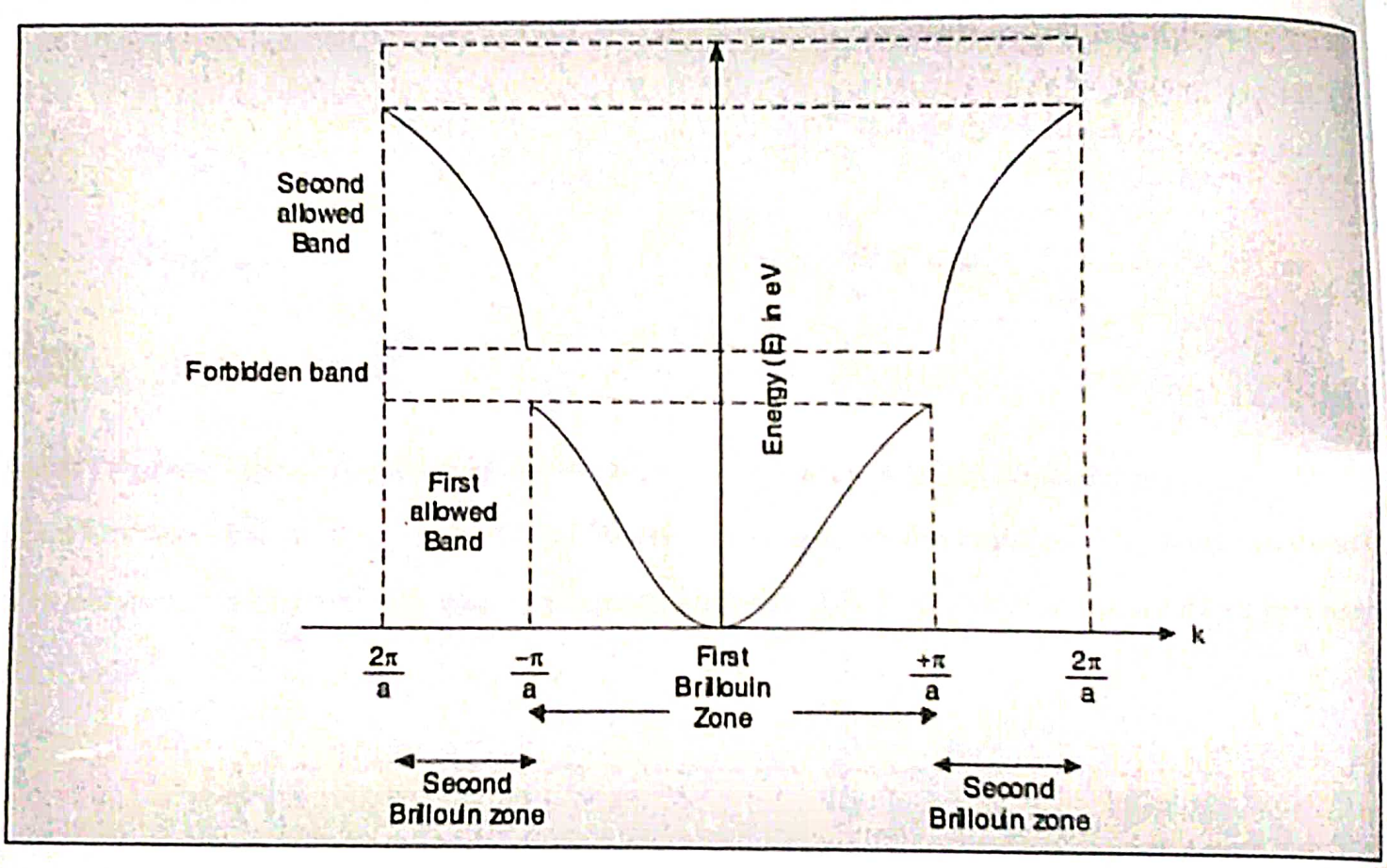


Fig. 1.58.

Two dimensional lattice : The first Brillouin Zone for a two dimensional lattice in X-Y plane is the square, the boundaries of which are given by the relation $k_x = \frac{+\pi}{a}$ and $k_x = \frac{-\pi}{a}$ and $k_y = \frac{+\pi}{a}$ and $k_y = \frac{-\pi}{a}$. The square drawn, whose boundaries are given by the relation

$$k_x = \pm \frac{2\pi}{a}, \; k_y = \pm \frac{2\pi}{a}$$

represent the second Brillouin Zone for a two dimensional lattice in the X-Y plane (Fig. 1.58). The square PQSR is the first Brillouin Zone. It is defined as the smallest volume enclosed by

the planes that are perpendicular bisectors of the reciprocal lattice vector drawn from the origin.

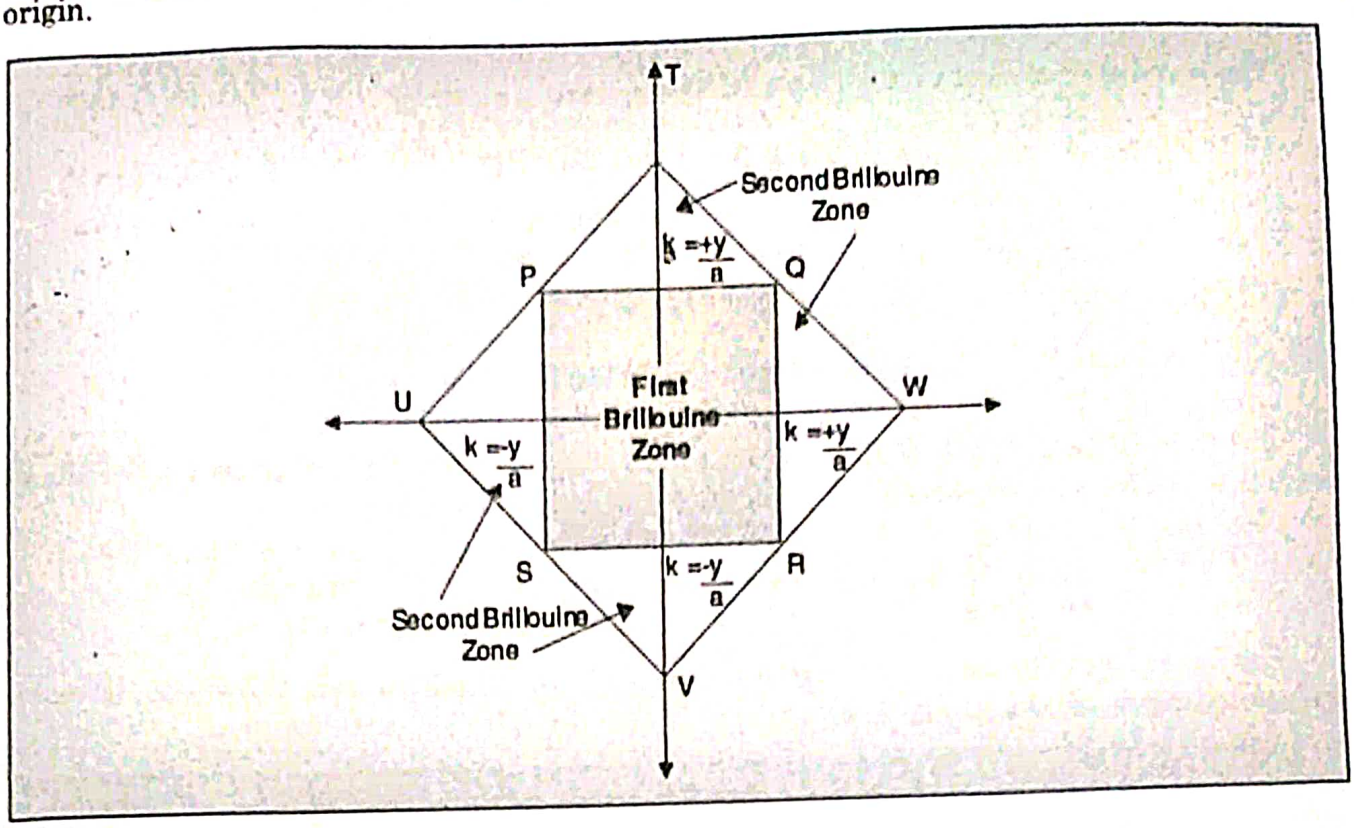


Fig. 1.58(a)

Brillouin Zone of Simple Cubic Lattice : The simple cubic lattice have the reciprocal primitive lattice vectors which are given as

$$\vec{A} = \frac{2\pi}{a}\hat{i},\ \vec{B} = \frac{2\pi}{a}\hat{j} \text{ and } \vec{C} = \frac{2\pi}{a}\hat{k}$$

The boundaries of first Brillouin Zone are the planes normal to $\vec{A}$, $\vec{B}$, $\vec{C}$, $-\vec{A}$, $-\vec{B}$ and $-\vec{C}$ and passing through mid points. These planes bound a cube of edge length $\frac{2\pi}{a}$. Thus the first Brillouin Zone of SC lattice is a cube and has volume $\left(\frac{2\pi}{a}\right)^3$. The second zone is made up of pyramids added to each face of the cube of first zone in the manner in which triangles are added to the first zone square in two dimensions. Similarly higher zones can also be constructed.

Brillouin Zone of Body Centered Cubic Lattice : The body centered cubic lattice have the reciprocal primitive lattice vectors which are given as

$$\vec{A} = \frac{2\pi}{a}(\hat{i} + \hat{j})$$

$$\vec{B} = \frac{2\pi}{a}(\hat{j} + \hat{k})$$

and $$\vec{C} = \frac{2\pi}{a}(\hat{i} + \hat{k})$$

The general reciprocal vector $\vec{G}$ for BCC structure is given by

$$\vec{G} = h\vec{A} + k\vec{B} + l\vec{C}$$

$$= \frac{2\pi}{a}[h(\hat{i} + \hat{j}) + k(\hat{j} + \hat{k}) + l(\hat{i} + \hat{k})]$$

$$= \frac{2\pi}{a}[(h + l)\hat{i} + (h + k)\hat{j} + (k + l)\hat{k}]$$

The first Brillouin zone of BCC lattice is the Wigner-Seitz cell formed by twelve planes normal to twelve vectors, which are in fact the shortest non-zero G's. *i.e.*

$$\frac{2\pi}{a}(\hat{i} \pm \hat{j}), \frac{2\pi}{a}(\hat{j} \pm \hat{k}) \text{ and } \frac{2\pi}{a}(\hat{i} + \hat{k})$$

The zone thus formed is a regular twelve faced primitive cell known as Rhombic dodecahedron as shown in Fig. 1.59.

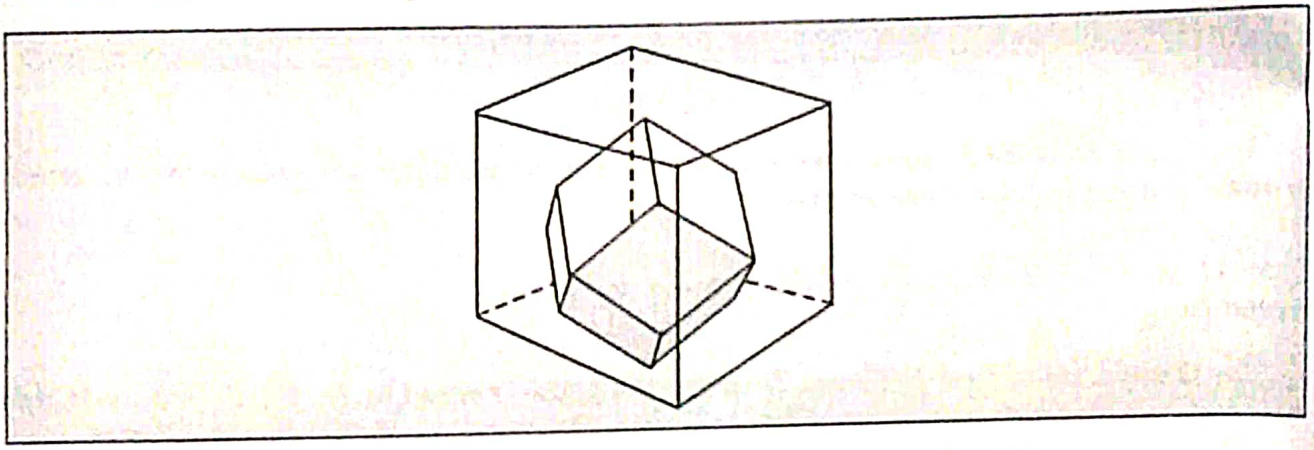


Fig. 1.59.

Point to Remember

Brillouin Zones form an essential part of the analysis of the electronic energy band structure of the crystals

Brillouin Zone of Face Centered Cubic Lattice : The face centered cubic lattice have the reciprocal primitive lattice vectors which are given by

$$\vec{A} = \frac{2\pi}{a}(\hat{i} + \hat{j} - \hat{k})$$

$$\vec{B} = \frac{2\pi}{a}(-\hat{i} + \hat{j} + \hat{k})$$

$$\vec{C} = \frac{2\pi}{a}(\hat{i} - \hat{j} + \hat{k})$$

The general reciprocal lattice vector $\vec{G}$ for BCC structure is

$$\vec{G} = h\,\vec{A} + k\,\vec{B} + l\,\vec{C}$$

$$= h\left[\frac{2\pi}{a}\left(\hat{i}+\hat{j}-\hat{k}\right)\right] + k\left[\frac{2\pi}{a}\left(-\hat{i}+\hat{j}+\hat{k}\right)\right] + l\left[\frac{2\pi}{a}\left(\hat{i}-\hat{j}+\hat{k}\right)\right]$$

$$= \frac{2\pi}{a}\left[(h+k-l)\,\hat{i} + (h+k-l)\,\hat{j} + (-h+k+l)\,\hat{k}\right]$$

Following eight vectors are the shortest non-zero G's

$$= \frac{2\pi}{a}\left(\pm\,\hat{i} \pm \hat{j} \pm \hat{k}\right)$$

The eight planes drawn perpendicular to the above eight vectors at their mid point do not make the closed primitive cell. The cell thus obtained by these planes is open at six square faces. The faces are the right bisectors of the following six reciprocal lattice vectors

$$\pm\left(\vec{A} + \vec{C}\right) = \frac{2\pi}{a}\left(\pm\,2\,\hat{i}\right)$$

$$\pm\left(\vec{A} + \vec{B}\right) = \frac{2\pi}{a}\left(\pm\,2\,\hat{j}\right)$$

and

$$\pm\left(\vec{B} + \vec{C}\right) = \frac{2\pi}{a}\left(\pm\,2\,\hat{k}\right)$$

So 14 planes make the first Brillouin Zone of FCC structure. These planes are the perpendicular bisectors of the following fourteen reciprocal lattice vectors.

$$\frac{2\pi}{a}\left(\pm\,\hat{i} \pm \hat{j} \pm \hat{k}\right),\ \frac{2\pi}{a}\left(\pm\,2\,\hat{i}\right),\ \frac{2\pi}{a}\left(\pm\,2\,\hat{j}\right) \text{ and } \frac{2\pi}{a}\left(\pm\,2\,\hat{k}\right)$$

Fig. 1.60 shows the first Brillouin Zone which has the shape of truncated octahedron.

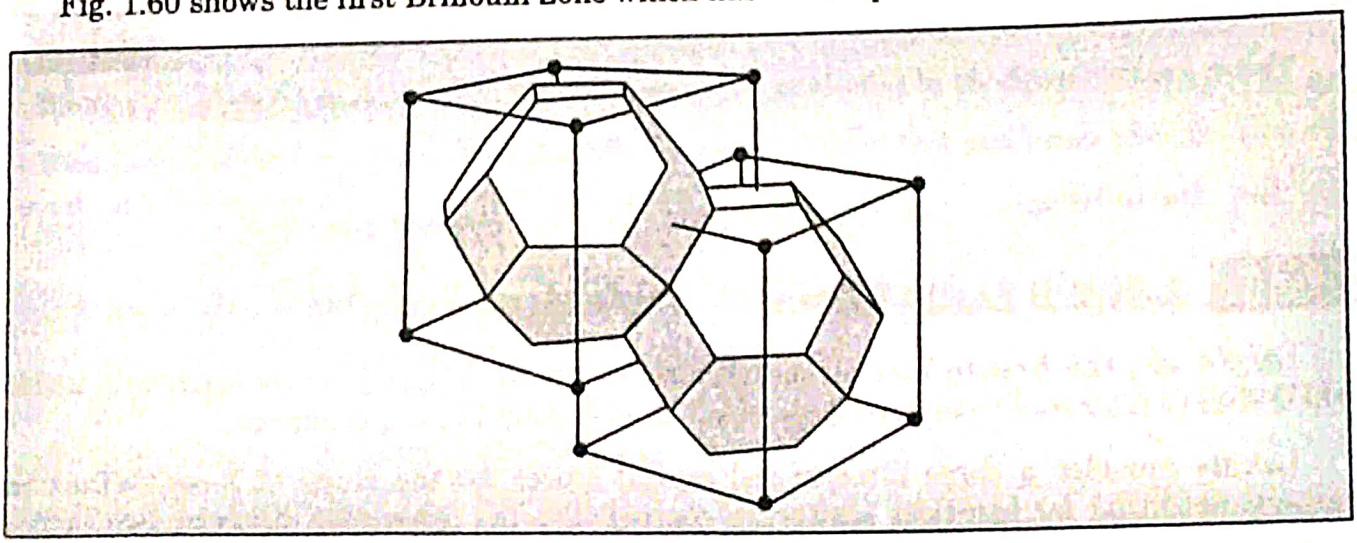


Fig. 1.60.

1.14 DIFFRACTION OF X-RAYS BY CRYSTALS

X-rays can be diffracted by crystals in the same way as the visible light is diffracted by a diffraction grating. So crystals can act like diffraction gratings. The idea that crystals can diffract X-rays was given by Von Laue, (1879-1960) a German physicist who won the Nobel Prize in Physics in 1914 for this discovery.

X-rays form part of the electromagnetic spectrum which were discovered by Roentgen in 1895. From the optical properties of X-rays, Sommerfeld (1868-1951) estimated that the wavelength of X-rays is about $10^{-10} m$. Crystallographers has estimated from a knowledge of density and molecular mass that spacing between two lattice points in a crystal is also about $10^{-10} m$. From these two physical facts it occurred to Max Von Laue that crystals serve as diffraction gratings for X-rays and show the phenomena of diffraction. He took the help of his colleagues Friedrich (1883-1968) and Knipping (1883-1935).

X-rays were used for demonstration of diffraction in crystals due to the fact that the wavelength of X-rays is comparable to the interatomic spacing in actual crystals. For example in sodium chloride (NaCl) crystal the atomic spacing is 2.8×10^{-10} m. Only X-rays which have wavelength close to 10^{-10} m can show diffraction. Visible or ultraviolet light has larger wavelengths and radiations of shorter wavelength like γ-rays are diffracted through very small angles which are difficult to measure.

Thus, a crystal diffracts X-rays because X-rays are scattered elastically without change of wavelength by the charged particles of the atoms in the crystal.

When X-rays fall on a crystal, the electrons present in the atoms start vibrating with a frequency equal to that of incident X-ray beam under the effect of the electric field of the radiation. These electrons undergo acceleration and the accelerated electrons emit secondary radiations of the same frequency as that of the incident X-rays. The secondary X-rays diffract in all directions. When X-rays have large wavelength equal to that of the atomic dimensions, all the radiations emitted by the electrons shall be in phase. On the other hand, if the incident X-rays have the same order of wavelength as that of the atomic dimensions, then the radiations emitted by the electrons are out of phase with one another. These radiations may, therefore exibit constructive or destructive interference producing maxima or minima in certain directions. Thus, crystal show diffraction pattern when X-rays fall on the crystals.

There are two methods of calculating the conditions of diffraction in crystals.

(i) due to Van Laue

(ii) due to Bragg

1.15 LAUE'S EQUATIONS

Laue's was the first to derive the diffraction equation which give the conditions under which X-rays scattered from the crystal combine to show a diffraction pattern.

Let us consider a three dimensional crystal lattice for the study of X-ray diffraction pattern produced by identical scattering centres. Let the separation between two lattice points L_1 and L_2 be $\vec{r}$. Allow a parallel beam of X-rays to fall on L_1 and L_2 as shown in Fig.

1.61. Let the incident beam be along the direction of unit vector $\hat{i}$. The X-ray beam on striking the lattice points, gets scattered along any arbitrary direction of unit vector $\hat{s}$. The scattered beam is also parallel beam of X-rays. Draw L_1N_1 and L_2N_2 perpendicular to the incident wave direction and scattered wave direction respectively to obtain incident wave front L_1N_1 and the scattered wave front L_2N_2. The path difference between the two scattered waves one scattered from L_1 and the other scattered from L_2 is given by

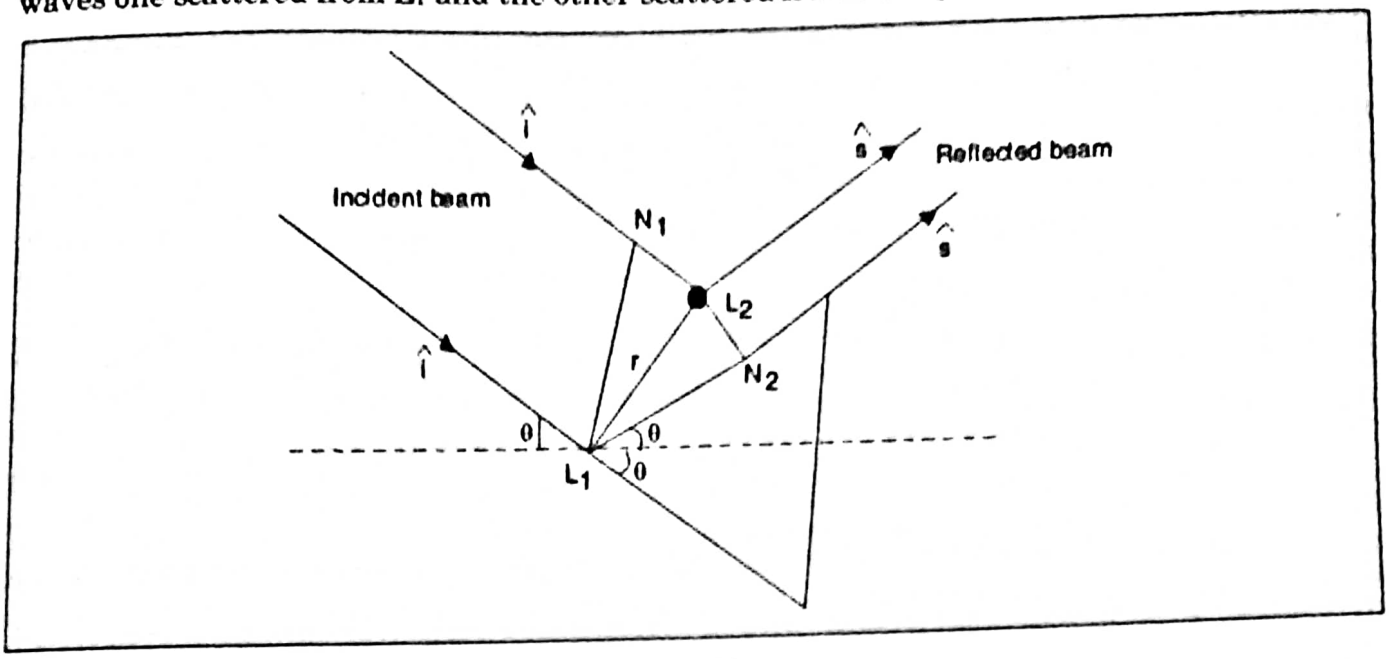


Fig. 1.61.

$$L_1N_1 - L_2N_2 = \vec{r} \cdot \hat{i} - \vec{r} \cdot \hat{s}$$

$$= \vec{r} \cdot (\hat{i} - \hat{s})$$

$$= \vec{r} \cdot \vec{N}$$

where $\vec{N}$ is a vector along the direction of the normal to the reflecting plane and $\vec{N} = (\hat{i} - \hat{s})$.

Let θ be the angle which the incident beam makes with the reflecting plane. The angle that the scattered beam of X-rays makes with the reflecting plane is also θ. The angle between the unit vectors $\hat{i}$ and $\hat{s}$ is 2θ. The magnitude of $\vec{N}$ is given by

$$| N | = 2 \sin \theta \qquad (\because \hat{i} \text{ and } \hat{s} \text{ are unit vectors})$$

If $\vec{r} \cdot N$ is the path difference, then the phase difference between the two scattered waves at lattice points L_1 and L_2 is given by

$$\phi = \frac{2\pi}{\lambda} (\vec{r} \cdot \vec{N})$$

1.58

For constructive interference to take place, the intensity of the diffracted beam is maximum when the phase difference ϕ is an integral multiple of 2π.

If $\vec{a}$, $\vec{b}$ and $\vec{c}$ are the primitive lattice vectors of the point L_2 with respect to the lattice point L_1 then,

$$\vec{r} = \vec{a} + \vec{b} + \vec{c}$$

The above condition of maxima will be satisfied if the following three conditions are also satisfied,

$$\phi_a = \frac{2\pi}{\lambda} (\vec{a} \cdot \vec{N}) = 2\pi h \quad \ldots(1)$$

$$\phi_b = \frac{2\pi}{\lambda} (\vec{b} \cdot \vec{N}) = 2\pi k \quad \ldots(2)$$

and

$$\phi_c = \frac{2\pi}{\lambda} (\vec{c} \cdot \vec{N}) = 2\pi l \quad \ldots(3)$$

where h, k and l are integers and ϕ_a, ϕ_b and ϕ_c are phase differences between the waves scattered from the two ends of the primitive lattice vectors $\vec{a}$, $\vec{b}$ and $\vec{c}$ respectively. If α, β and γ be the angles between the normal to the reflecting plane and $\vec{a}$, $\vec{b}$ and $\vec{c}$ axes respectively, then,

$$\vec{a} \cdot \vec{N} = |\vec{a}| \, |\vec{N}| \cos\alpha$$

$$= 2a \sin\theta \cos\alpha$$

$$\vec{b} \cdot \vec{N} = |\vec{b}| \, |N| \cos\beta$$

$$= 2b \sin\theta \cos\beta$$

$$\vec{c} \cdot \vec{N} = |\vec{c}| \, |N| \cos\gamma$$

$$= 2c \sin\theta \cos\gamma$$

From equations (1), (2) and (3) we have,

$$\vec{a} \cdot \vec{N} = h\lambda$$

$$\vec{b} \cdot \vec{N} = k\lambda$$

and

$$\vec{c} \cdot \vec{N} = l\lambda$$

Therefore,

$$2a \sin\theta \cos\alpha = h\lambda \quad \ldots(4)$$

$$2b \sin\theta \cos\beta = k\lambda \quad \ldots(5)$$

$$2c \sin\theta \cos\gamma = l\lambda \quad \ldots(6)$$

The equations (4), (5) and (6) are known as Laue's equation for X-ray diffraction.

Point to Remember

Laue's theory is also known as the geometrical theory of X-ray diffraction.

1.16 BRAGG'S LAW

When X-rays are allowed to fall on a crystal lattice, peaks of scattered intensity are observed which follow the following conditions

(i) The angle of incidence = angle of scattering.

(ii) The path difference is an integral multiple of the wavelength.

William Lawrence Bragg (1890 – 1971) and his father William Henry Bragg (1862 – 1942) provided another interpretation in 1912. They assumed that the X-rays are reflected at atomic planes. The result was similar to that of Laue's result for diffraction of X-rays by crystals. Braggs were awarded Nobel Prize in physics in 1915.

Point to Remember

Laue did not start with the assumption that X-rays are reflected. Instead, he assumed that they were scattered by the atoms in the crystal.

Consider parallel lattice planes spaced at a distance 'a' as shown in Fig. 1.62. Let the Miller indices be (h k l) and a parallel beam of X-rays of wavelength λ be incident a glancing angle θ such that the ray lies along the plane of the paper. Let two rays MA and NB be incident at point A and B and the reflected rays pass along AO and BP. Draw AQ and AR perpendiculars on NB and BP respectively.

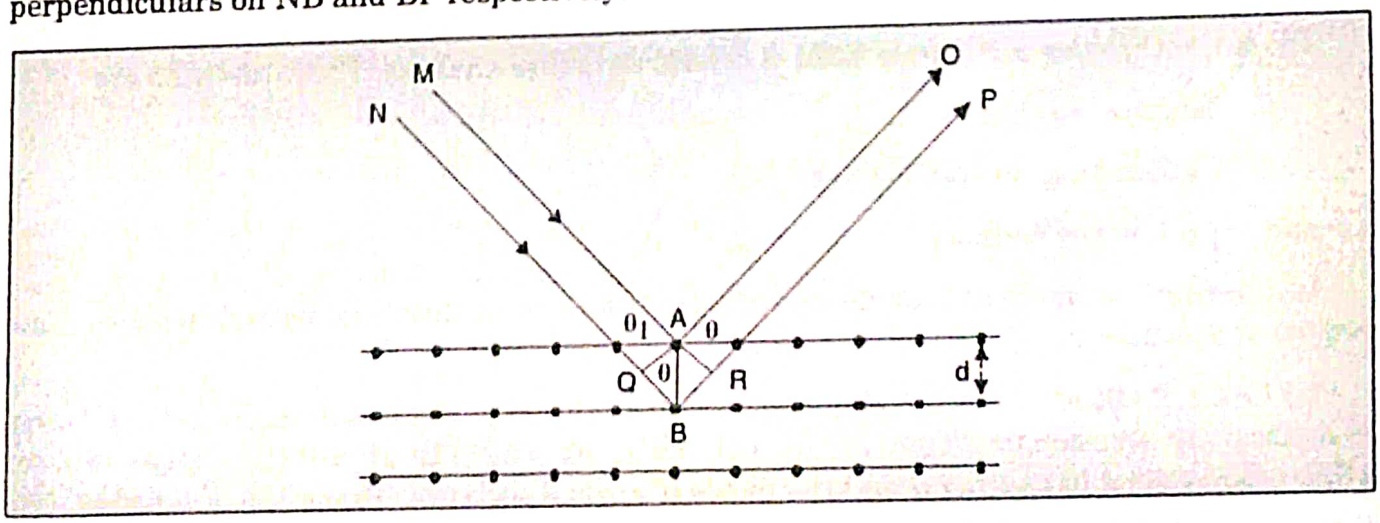


Fig. 1.62.

According to the principle of interference of waves, constructive interference takes place whenever the path difference between rays reflected from the adjacent planes is an integral multiple of wavelength λ. Here, the path difference is (QB + BR)

i.e. $$QB + BR = n\lambda$$

Now from the Fig. 1.62,

$$QB = BR = d \sin\theta$$

where θ is the angle of incidence as well as the angle of reflection which is called glancing angle.

Thus,

$$2d \sin\theta = n\lambda$$

where $n = 1, 2, 3, 4, \ldots\ldots$

If $n = 1$ it is first order. For $n = 2$, we have second order maxima and so on. The above equation is known as Bragg's Law.

Point to Remember

The Bragg's law is a consequence of the periodicity of crystal lattice. The law does not give any idea about the arrangement of atoms in the basis.

The composition of basis determines the relative intensity of the various orders of diffraction from a given set of parallel planes. From Bragg's law it is obvious that in order to get diffraction effects, $\lambda \leq 2d$ otherwise the law will not hold good. Hence, with long wavelength the Bragg's law does not operate. Because of this the Bragg's reflection with visible light is not possible. The maximum value of d is the lattice parameter a which is of the order of 4×10^{-10} m.

1.17 EXPERIMENTAL X-RAY DIFFRACTION METHODS OF CRYSTALS

When X-rays fall on a single crystal, then Bragg's law requires that wavelength λ and glancing angle θ must be matched. Thus to satisfy Bragg's law it is necessary to change either λ or θ.

There are three important methods of crystal structure analysis. These methods are

(i) Laue method

(ii) Rotating crystal method

and (iii) Powder method

In the first two methods, single crystals are used and in the third method, we use a fine powdered specimen.

(i) Laue Method : In this method a single crystal is kept stationary in the path of X-rays of continuous wavelength. The crystal will select out and diffract discrete values of λ for which planes exist of spacing d and the incident angle θ such that Bragg law is satisfied. The dimensions of the crystal are 1 mm × 1 mm × 1 mm and the wavelength of X-rays vary from 0.2 to 2 A°. We place a flat photographic film to receive either the transmitted or reflected diffraction beam. The experimental arrangement is shown in Fig. 1.63. The Goniometer is an instrument which measure angles accurately.

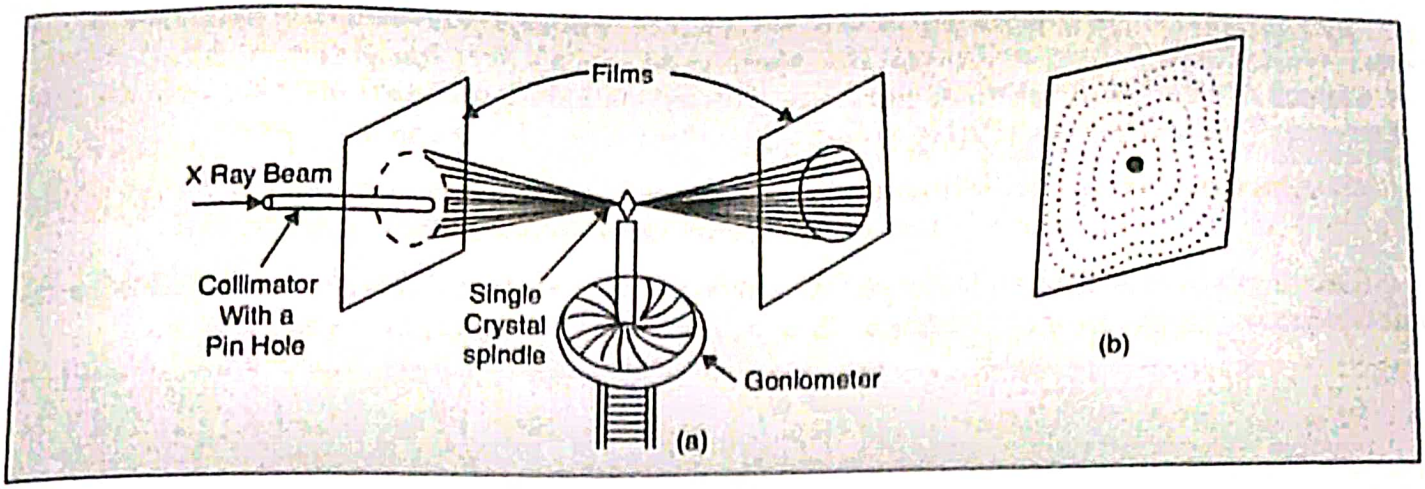


Fig. 1.63.

A series of spots are obtained on the screen which represent a diffraction pattern (Fig. 1.63 (b)).

Hence the Laue method helps us to study the symmetry of the crystal lattice. The orientation of planes, which were, cut from a crystal at unknown angles to the elements of symmetry of the crystal, were also determined using this method.

Laue method is not useful for the deduction of crystal structure. This is due to the fact that out of the wide range of wavelengths it is possible for the several wavelengths to reflect in different orders from a single plane so that the different orders of reflection may superpose a single Laue spot. Because of this the measurement of the reflection intensity of individual spots becomes difficult.

(ii) Rotating Crystal Method : In this method a single crystal is rotated about a fixed axis and monochromatic beam of X-rays is used. The crystal used has the dimensions of 1 mm. The experimental set up shown in Fig. 1.64 has a cylindrical film whose axis coincides with the axis of rotation of the crystal. The X-ray pattern is depicted on this film. The diffraction pattern is formed from the planes which obey Bragg's law.

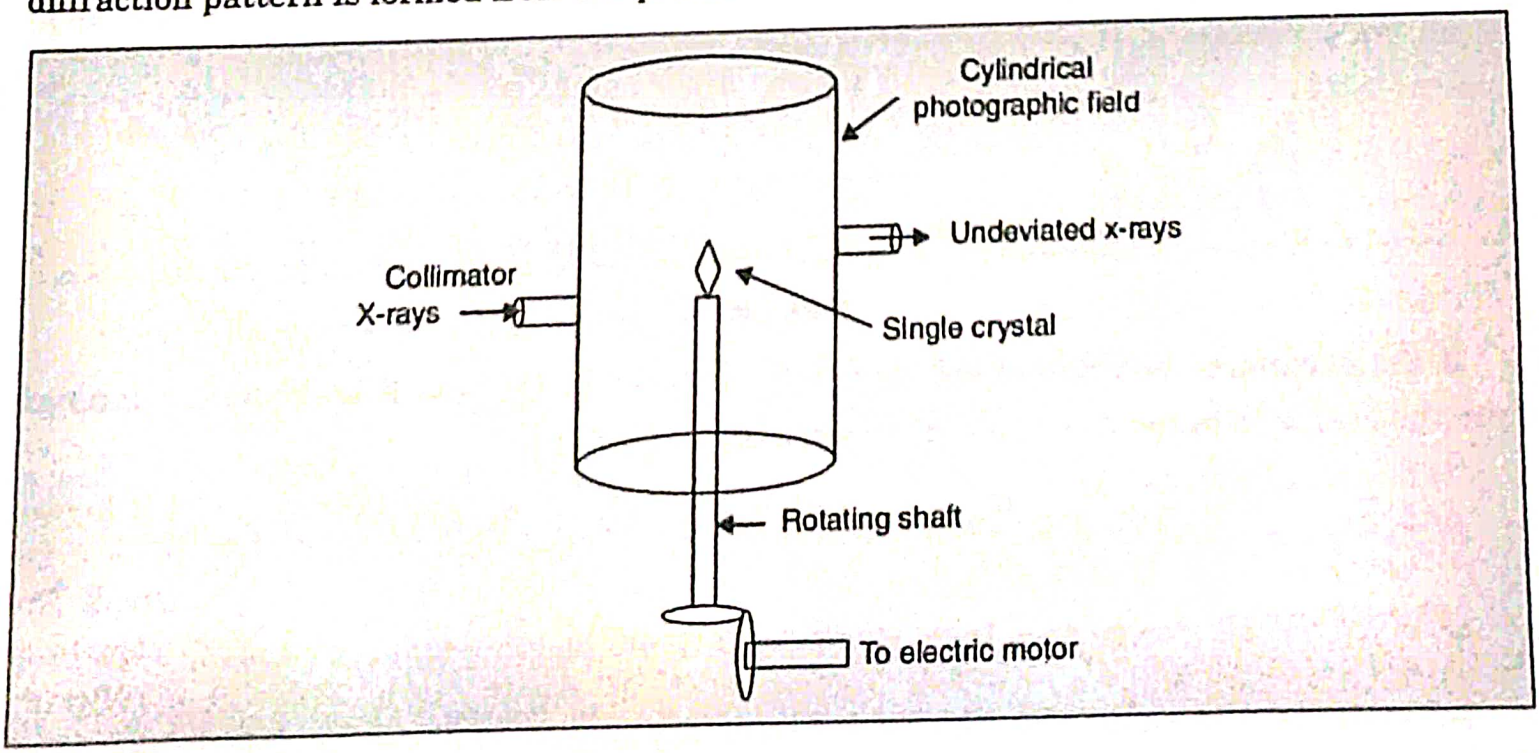


Fig. 164.

The crystal can be rotated in two ways. One way of rotation is complete rotation and the other way is an oscillatory rotation. This method requires a very small crystal which rotates at a speed of 10 to 15 revolutions per hour. The axis of rotation should coincide with an edge of crystal. This method is useful in determining the values of a, b and c of a crystal.

(iii) Powder Method : In this method, a powdered specimen is packed in a thin walled capillary which is held on a movable mount at the centre of cylindrical camera.

This method was used by Debye (1884-1966) and his student Scherrer (1890-1969) for the determination of the crystal structure. The experimental set up is shown in Fig. 1.65.

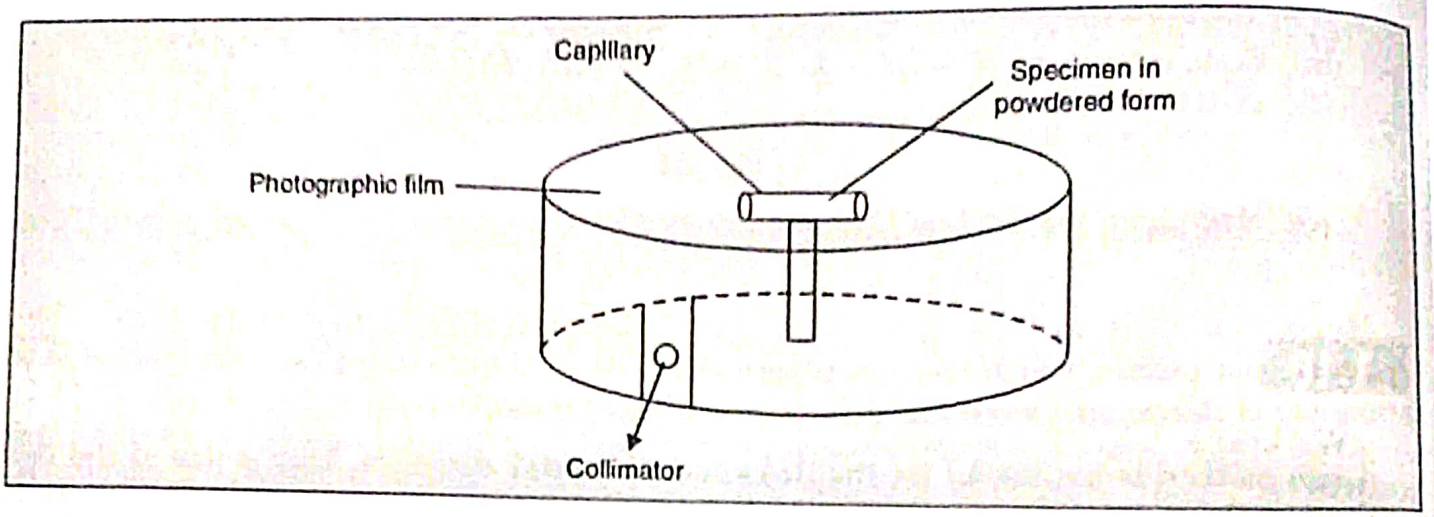


Fig. 1.65.

The monochromatic X-rays strike the powdered specimen. On the inner side of a cylindrical chamber a photographic film is wrapped. The specimen contains micro crystals which are to be oriented with planes making a Bragg angle θ with the beam. Diffracted beam from a large number of micro crystals, which are randomly oriented are produced making an angle 2θ with the incident beam. Therefore, the collection of all such diffracted beams gives a cone of semi angle 2θ. Diffraction pattern of the crystals is shown in Fig. 1.66.

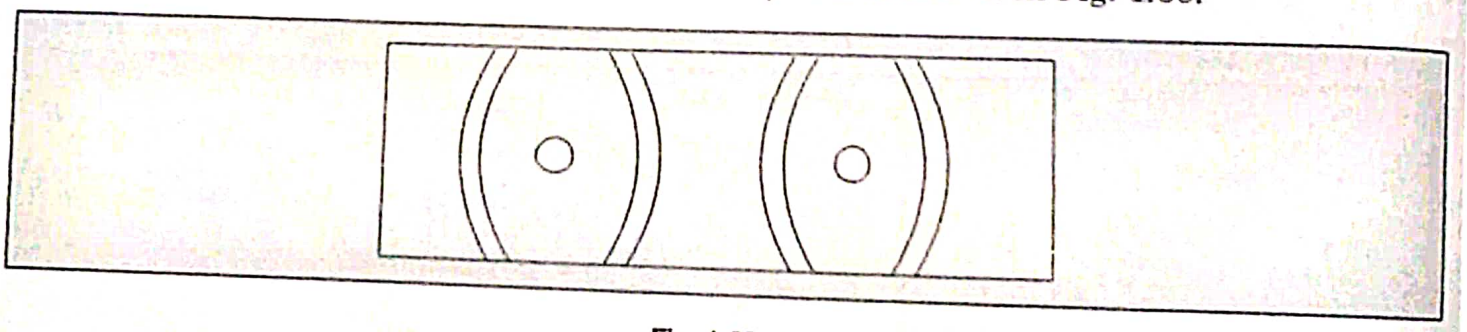


Fig. 1.66.

If the maximum diameter of the ring in the pattern is D_m and R is the radial distance from the specimen to the film then the Bragg's law is given by

$$\theta = \frac{D_m}{4R}$$

or

$$D_m = 4R\theta$$

By knowing, the value of θ, the inter planer distance 'd' can also be determined using Bragg's law.

The main advantage of the powder method is that any material can be broken into powder and we do not have to take a large single crystal. This method also helps to solve many important problems given below :

(i) If photographs are made before and after treatment such as by heat, mechanical or any other, of a crystalline substance, their comparisons reveals any changes in the lattice.

(ii) Distinction between a crystalline material and amorphous material can be made. A crystalline material produces lines on a photograph whereas no lines are produced on a photograph of an amorphous material.

(iii) A mineral can be determined if its powder photograph is compared with the standard photographs in a mineralogical determinative manual.

(iv) The size of unit cell and the type of the lattice can be determined using this method.

(v) With the help of standard photographs of known chemical compounds their presence may be detected in an unknown mixture.

1.18 BRILLOUIN ZONES IN RECIPROCAL LATTICE

We know that a Brillouin Zone is the collection of all those k-values in the reciprocal lattice which are Bragg reflected. Now, let us construct a Brillouin Zone for simple square lattice of side a.

The primitive translation vectors of this lattice are given as

$$\vec{a} = a\,\hat{i}$$

$$\vec{b} = b\,\hat{j}$$

The translation vectors of reciprocal lattice becomes,

$$\vec{A} = \left(\frac{2\pi}{a}\right)\hat{i}$$

and

$$\vec{B} = \left(\frac{2\pi}{a}\right)\hat{j}$$

Hence the reciprocal lattice vector $\vec{G}$ is given by

$$\vec{G} = h\,\vec{A} + k\,\vec{B}$$

$$= \frac{2\pi}{a}\,[h\,\hat{i} + k\,\hat{j}]$$

where h and k are integers and the wave vector $\vec{k}$ is expressed as

$$\vec{k} = k_x\,\hat{i} + k_y\,\hat{j}$$

According to Bragg's condition

$$2\,\vec{k}\,.\,\vec{G} + G^2 = 0$$

or $$2\,(k_x G_x + k_y G_y) + G_x^2 + G_y^2 = 0$$

or $$2\left[k_x \frac{2\pi}{a} h + k_y \frac{2\pi}{a} k\right] + \left(\frac{2\pi}{a}\right)^2 h^2 + \left(\frac{2\pi}{a}\right)^2 k^2 = 0$$

or $$\frac{4\pi}{a}\,(hk_x + kk_y) = -\left(\frac{2\pi}{a}\right)^2 (h^2 + k^2)$$

or $$hk_x + kk_y = \frac{-\pi}{a}\,(h^2 + k^2)$$

This equation represents a family of straight lines in the k_x and k_y plane. Their k_x and k_y intercepts are given by the equations

$$k_x = -\frac{\pi}{a}\,\frac{(h^2 + k^2)}{h}$$

and $$k_y = -\frac{\pi}{a}\,\frac{(h^2 + k^2)}{k}$$

By taking all possible combinations of h and k, we can obtain the values of $\vec{k}$

For $h = \pm 1$ and $k = 0$,

$$k_x = \pm\frac{\pi}{a} \text{ and } k_y \text{ is arbitrary}$$

For $h = 0$ and $k = \pm 1$,

k_x is arbitrary and $k_y = \pm\dfrac{\pi}{a}$

The graph of these four lines

$$k_x = +\frac{\pi}{a},\ k_x = -\frac{\pi}{a},\ k_y = +\frac{\pi}{a} \text{ and } k_y = \frac{-\pi}{a}$$

is plotted in Fig. 1.67. The first Brillouin Zone is produced by taking origin at 0, the Bragg reflection is produced by taking all the k-vectors originating from origin and terminating on these lines. The square bounded by $k_x = \pm\left(\dfrac{\pi}{a}\right)$ and $k_y = \pm\left(\dfrac{\pi}{a}\right)$ is the first Brillouin Zone.

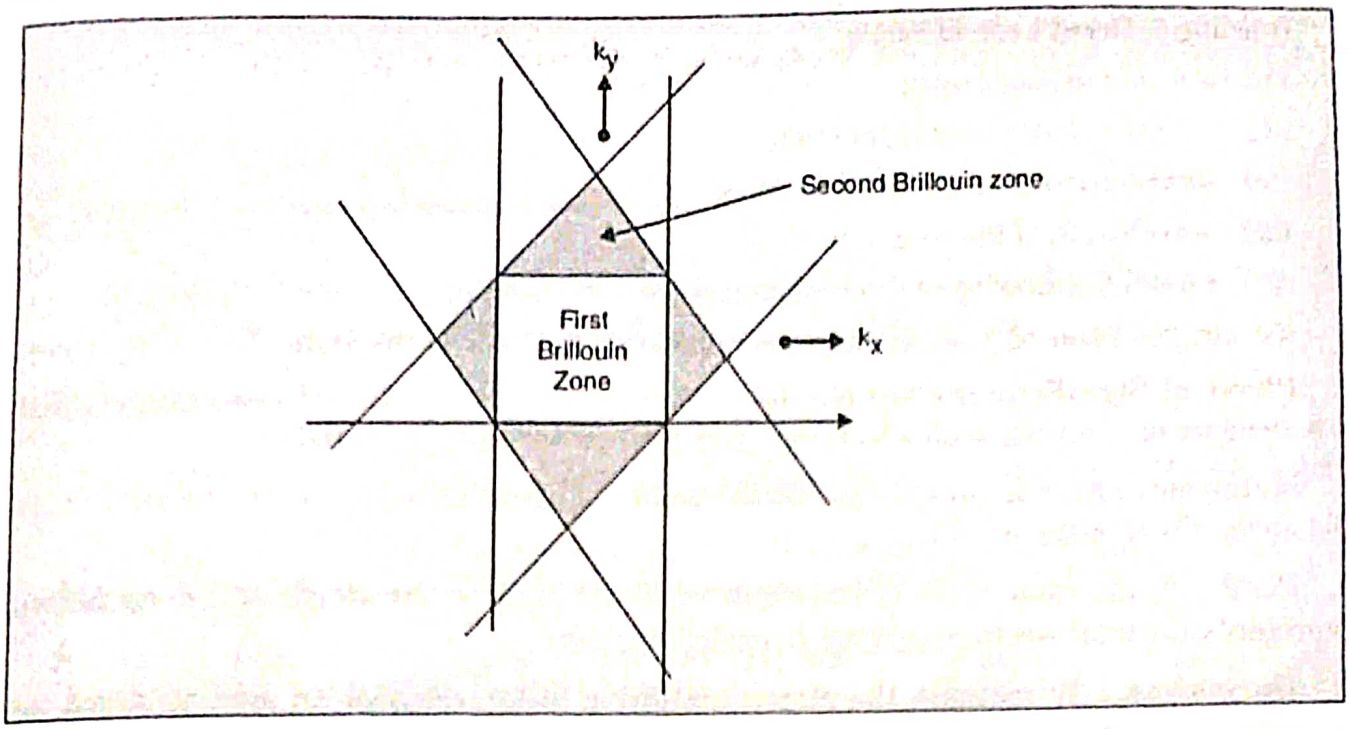


Fig. 1.67.

For $h = \pm 1$ and $k = \pm 1$, we have

$$\pm k_x \pm k_y = \frac{2\pi}{a}$$

or

$$k_x + k_y = \frac{+2\pi}{a}$$

$$k_x + k_y = \frac{-2\pi}{a}$$

$$k_x - k_y = \frac{+2\pi}{a}$$

$$k_x - k_y = \frac{-2\pi}{a}$$

The additional area shown as shaded in Fig. 1.67 is bound by these four lines represent the second Brillouin Zone and similarly the third, fourth and other zones can be constructed.

Point to Remember

A k-vector that does not terminate on a zone boundary cannot produce a Bragg reflection.

1.19 ATOMIC SCATTERING FACTOR

The ratio of the amplitude of radiations scattered from an atom to the amplitude of radiations scattered from an electron is called **Atomic Scattering Factor** (f).

$$i.e. \quad f = \frac{\text{Amplitude of radiation scattered from an atom}}{\text{Amplitude of radiation scattered from an electron}}$$

It is also referred as form factor.

The value of f depends upon

(i) number of electrons in an atom

(ii) distribution of electrons in an atom

(iii) wavelength of the radiation wave

(iv) angle of scattering of the radiation wave

Usually the value of 'f is less than the number of electrons in the atom.

Physical Significance : The physical significance of the atomic scattering factor is that it a measure of efficiency with which the atom scatters the incident radiation.

Mathematically, f is equal to the total number of electrons Z present in the atom when the angle of scattering is zero.

For $\theta > 0$, the value of $f < Z$. In simple words we say that the atomic scattering factor represents the total electronic charge Z inside the atom.

Derivation : To measure the atomic scattering factor, consider an atom in which the incident and reflected wave normals are at equal angles θ with the normal N to the reflecting plane at point O, the centre of the atom as shown in Fig. 1.68.

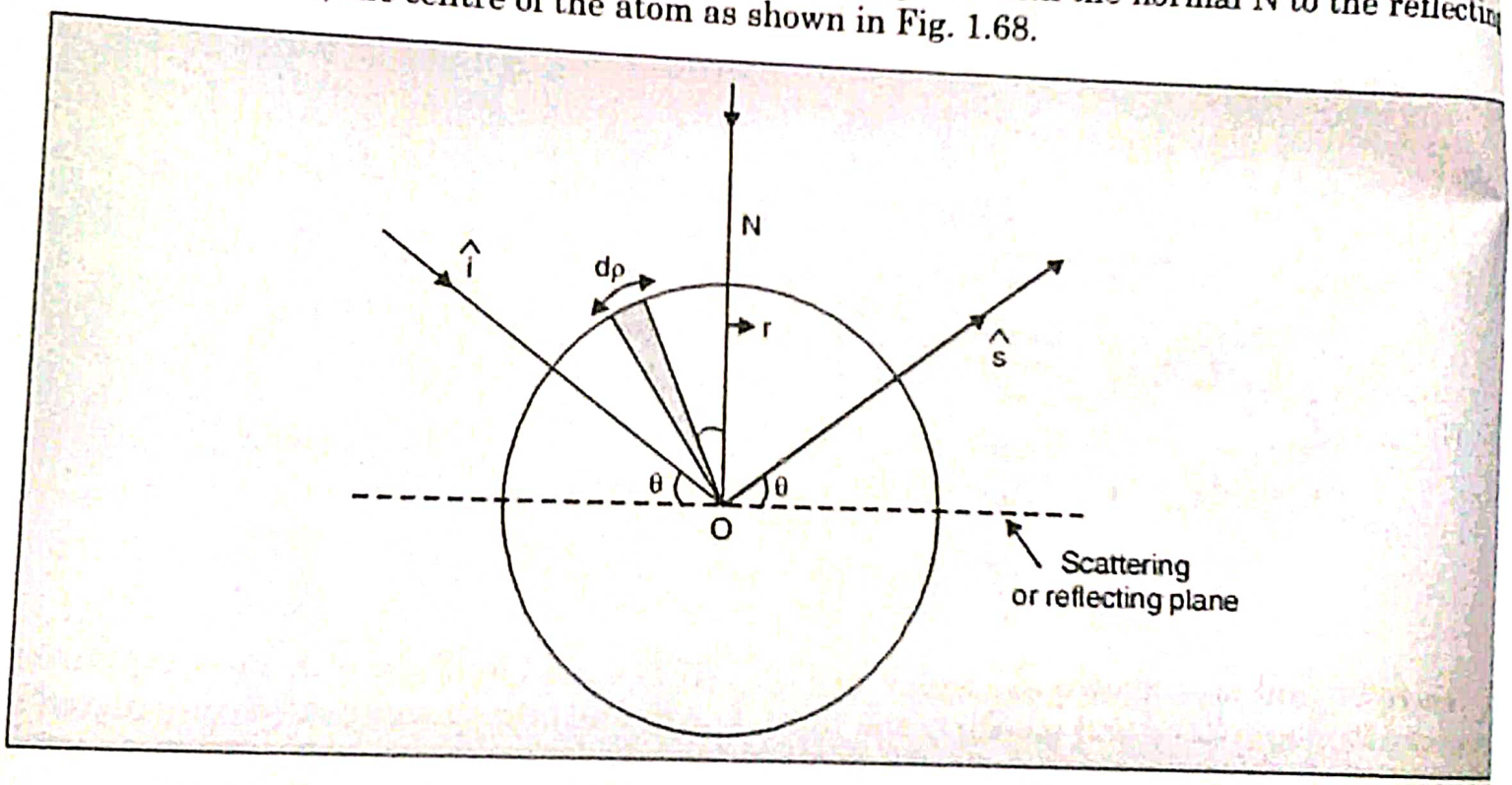


Fig. 1.68.

Let an elementary segment of charge $\rho(r)\, dV$ is considered in a small volume dV placed at the position $(\vec{r}, \phi)$. The quantity $\rho(r)$ determines the contribution of atom to the concentration of electron at $\vec{r}$. The quantity $\rho(r)\, dV$ gives the probability of finding the electron in the element of volume dV at r. The phase difference ϕ between the radiation scattered at the origin and that scattered in the volume element dV at r is given by

$$\phi = \frac{2\pi}{\lambda} (\vec{r} \cdot \vec{N})$$

If the scattering amplitude from the electron along the direction of unit vector $\hat{s}$ is represented by $A\ e^{i(kx - \omega t)}$

where $k = \frac{2\pi}{\lambda}$, x is a distance along the scattering direction $\hat{s}$.

The amplitude of the scattered wave from the small elementary segment of volume element dV having a phase difference ϕ is given by

$$A\ e^{i[(kx - \omega t) + \phi]}\ \rho(r)\ dV$$

Then, by definition the ratio of the amplitude of the radiation scattered to the element of charge $\rho(r)\ dV$ at $\vec{r}$ to that scattered by a point electron at the centre O of the atom (*i.e.* origin) is given by small change in atomic scattering factor df,

$$df = \frac{A\ e^{i[(kx - \omega t) + \phi]}\ \rho(r)\ dV}{A\ e^{i(kx - \omega t)}}$$

$$= e^{i\phi}\ \rho(r)\, dV$$

$$= e^{i\left(\frac{2\pi}{\lambda}\right)(\vec{r}\ .\ \vec{N})}\ \rho(r)\, dV \qquad \ldots(*)$$

Now we know that

$$\vec{r}\ .\ \vec{N} = |\ r\ |\ |\ N\ |\ \cos\phi$$

$$= 2\, r \sin\theta \cos\phi$$

(Refer art 1.13 Laue's equation)

Hence

$$\frac{2\pi}{\lambda}\ (\vec{r}\ .\ \vec{N}) = \frac{4\pi}{\lambda}\ r \sin\theta \cos\phi$$

$$= M\, r \cos\phi$$

where $$M = \frac{4\pi}{\lambda} \sin\theta$$

Also $$dV = 2\pi\ r^2 \sin\phi\, d\phi\, dr$$

is the volume of an elementary ring of radius $r \sin\phi$, width $r\, d\phi$ and thickness $d\vec{r}$.

Integrating the equation (*), we get the atomic scattering factor f

$$f = \int df$$

$$= \int_{r=0}^{\infty} \int_{\phi=0}^{\pi} \rho(r)\ e^{iMr\cos\phi}\ 2\ \pi\ r^2\ \sin\ \phi\ d\ \phi\ dr$$

On solving the integral

$\int_0^{\pi} e^{iMr\cos\phi}\, d\phi$, we obtain

$$\int_0^{\pi} e^{iMr\cos\phi}\, d\phi = \frac{2\sin Mr}{Mr}$$

Hence,

$$f = \int_0^{\infty} 4\pi r^2 \rho(r)\, \frac{\sin Mr}{Mr}\, dr$$

When θ approaches zero, M approaches zero then $\frac{\sin Mr}{Mr}$ will approach unity.

Therefore,

$$\underset{M\to 0}{\text{Lt}}\ f = \int_0^{\infty} 4\pi r^2 \rho(r) dr$$

= Total number of electrons in the atom

= Z (the atomic number of the element)

Thus the atomic scattering factor is numerically equal to the total number of electrons (Z) in the atom.

1.20 GEOMETRICAL STRUCTURE FACTOR

Geometrical structure factor is defined as the ratio of the amplitude of the wave scattered by an entire unit cell to the amplitude of the wave scattered by a single point electron for the same wavelength at the origin.

The intensity of a beam scattered from a crystal depends upon

(i) the atomic scattering factor of the atoms

(ii) number of atoms in the unit cell

(iii) type of atoms in the unit cell

(iv) distribution of atoms in the unit cell

Because of path difference covered by X-rays after reflection from different atoms, the total intensity of scattered beam from a unit cell is not equal to number of atoms times the intensity of beam scattered by atom.

Mathematically, geometrical structure factor is defined as the ratio of the total scattering amplitude F($h\ k\ l$) to the atomic scattering factor f.

$$\text{Geometrical structure factor } \xi = \frac{\text{Total scattering amplitude F(h k l)}}{\text{Atomic scattering factor } (f)}$$

Derivation : Suppose there are n number of atoms in the unit cell of the crystal. The

basis, which forms a group of atoms attached to lattice point is repeated in space to form the crystal structure. The number of atoms in a basis may be few in many metals and inert gases but can be large in some elements.

The position of any arbitrary atom *j*th of the cell is written as

$$\vec{r_j} = x_j \vec{a} + y_j \vec{b} + z_j \vec{c}$$

The position is so arranged that the coordinates x_j, y_j, and z_j lie between 0 and 1

If f_j be the atomic scattering factor of *j*th atom, then the total scattering amplitude of the crystal for a given $(h\ k\ l)$ reflection is

$$F(h\ k\ l) = \sum_{j=1}^{n} f_j \ e^{i\phi_j}$$

where ϕ_j is the phase difference between the wave scattered at origin and that scattered from the atom. It is given as

$$\phi_j = \frac{2\pi}{\lambda} (\vec{r_j} \cdot \vec{N})$$

where $\vec{r_j}$ is the position vector from the *j*th atom to the origin and N is a vector normal to the reflecting plane

Let us expand $(\vec{r_j} \cdot \vec{N})$

$$(\vec{r_j} \cdot \vec{N}) = x_j \vec{a} + y_j \vec{b} + z_j \vec{c}) \cdot \vec{N}$$

$$= x_j (\vec{a} \cdot \vec{N}) + y_i (\vec{b} \cdot N) + z_j (\vec{c} \cdot \vec{n})$$

Bur $\vec{a} \cdot \vec{N} = h\lambda$

$\vec{b} \cdot \vec{N} = k\lambda$

and $\vec{c} \cdot \vec{N} = l\lambda$

Therefore, $|F(h\ k\ l)| = \sum f_j e^{i2\pi(hx_j + ky_i + dz_j)}$

If all the atoms are similar in a cell, then f_j will be same for all the atoms

$$F(h\ k\ l) = f\xi$$

or $$\xi = \frac{F(hkl)}{f}$$

Physical Significance : The physical significance of geometrical structure factor ξ is that there is no intensity at reflection N allowed by the space lattice corresponding to zero value of ξ. The missing reflections help us to determine the structure of the lattice of the crystal. The geometrical structure factor may not be real.

The intensity of radiation is proportional to the square of its amplitude. The intensity of the scattered radiation can be expressed as

$$I = | F |^2$$

$$= FF^*$$

where F^* is the complex conjugate of F.

Hence, the intensity I is given as

$$I = \left[\sum f_j \cos 2\pi (hx_j + ky_j + lz_j)\right]^2$$

$$+ \left[\sum_j f_j \sin 2\pi (hx_j + ky_j + lz_j)\right]^2$$

For SC Crystal : There is only one atom per unit cell at the origin, therefore,

$$x_j = y_j = z_j = 0$$

and $$F(h\,k\,l) = f$$

Hence all the lines predicted by Bragg's law will occur, provided f is sufficiently large to make the peaks of intensity visible.

For BCC Crystal : There are two identical atoms per unit cell one contributed by the corner atoms of the cell and the other at the centre of the cell. Let $x_1 = y_1 = z_1 = 0$ for the corner atom. The other atom in the cell is the body centre atom which belongs to the unit cell and its coordinate are $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$. Hence geometrical structure factor ξ of body centered cubic lattice becomes

$$\xi = f\left[\sum_j e^{i\,2\pi\,(hx_j + ky_j + lz_j)}\right]$$

$$= f\left[1 + e^{\pi i(h+k+l)}\right]$$

Here, we have put $x_i = y_i = z_i = 0$ for the first term

and $x_i = y_i = z_i = \frac{1}{2}$ for the second term

For any ($h\ k\ l$) reflection for which ($h + k + l$) is an odd integer, the term $e^{-i\pi(h+k+l)} = -1$

For any ($h\ k\ l$) reflection for which ($h + k + l$) is an even integer, the term $e^{i\pi(h+k+l)} = 0$

Hence

$$F(h\ k\ l) = f(1 - 1)$$

$$= 0 \qquad \text{(for an odd integer)}$$

where f is the atomic form factor.

Similarly

$$F(h\ k\ l) = f(1 + 1)$$

$$= 2f \qquad \text{(for an even integer)}$$

Therefore first order reflection for BCC structure, does not take place from the planes like (100), (300) (111), (221) etc. but will occur from the planes like (200), (110), (222) etc.

For FCC Crystal : The basis for the face centered cubic structure has four identical atoms per unit cell, one contributed by the corner atoms and three contributed by the face centre atoms. The four atoms are positioned at coordinates

$$(000),\ \left(0\ \frac{1}{2}\ \frac{1}{2}\right),\ \left(\frac{1}{2}\ 0\ \frac{1}{2}\right) \text{ and } \left(\frac{1}{2}\ \frac{1}{2}\ 0\right)$$

Thus the diffraction amplitude for the ($h\ k\ l$) reflection is given by

$$F(h\ k\ l) = f\left[1 + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(l+h)}\right]$$

For all even or odd indices, $h\ k\ l$, then the amplitude

$$F(h\ k\ l) = f(1 + 1 + 1 + 1)$$

$$= 4f$$

and so the intensity is proportional to $(4f)^2$

i.e. $16f^2$

If one of the indices say h = odd and other two are even, then

$$e^{\pi i(h+k)} = -1$$

$$e^{\pi i(l+h)} = -1$$

and $$e^{\pi i(k+l)} = -1$$

Then $$F(h\ k\ l) = f(1 - 1 - 1 + 1)$$

$$= 0$$

and so the intensity is zero. Also, if one of the indices is even and other two are odd, then $F(h\ k\ l)$ is zero and so the intensity is also zero.

Hence in an FCC structure no reflection can take place for which the integers are partly even and partly odd.

SOLVED PROBLEMS

Problem 1. **The radius of an atom of FCC structure is 122 pico metre. What is the edge length of the unit cell of that atom's lattice ?**

Solution :

Let us suppose that edge length of unit cell is a and radius of an atom is r, then the edge length of unit cell of FCC atom is

$$a = (2\sqrt{2})r$$

$$= 2\ (\sqrt{2})\ (122 \times 10^{-12})$$

$$= 345.01 \times 10^{-12}\ \text{m}$$

$$= 345.01\ \text{pm}$$

Problem 2. **Find the Miller indices of a set of parallel planes which make intercepts in the ratio of $3a : 4b$ on the X and Y axis and are parallel to Z-axis, where $\vec{a}$, $\vec{b}$ and $\vec{c}$ are the primitive lattice vectors.**

Solution :

Intercept on the X-axis = $3a$

Intercept on the Y-axis = $4b$

Intercept on the Z-axis = ∞, because the set of planes is parallel to Z-axis.

The reciprocal of the numbers 3, 4 and ∞ are $\frac{1}{3}$, $\frac{1}{4}$ and $\frac{1}{\infty}$

The LCM of the denominators is 12. Multiply above ratios by LCM 12.

Thus, the smallest three integers having the same ratio are 4, 3, 0

Hence Miller indices ($h\ k\ l$) = **(430)**

Problem 3. **Find the Miller indices if the given plane makes intercept of 1A°, 2Å and 3Å on the axes of the crystal for which lattice parameters are $a = 2$, $b = 1$ and $c = 3$.**

Solution :

Given, $a : b : c = 2 : 1 : 3$

If the intercepts are

$$n_1 a = 1\text{Å}$$

$$n_2 b = 2\text{Å}$$

$$n_3 c = 3\text{Å}$$

then the numbers n_1, n_2 and n_3 are

$$n_1 = \frac{1}{a} = 1$$

$$n_2 = \frac{2}{b} = \frac{2}{2} = 1$$

$$n_3 = \frac{3}{c} = \frac{3}{3} = 1$$

Reciprocals of these intercepts are

$$\frac{1}{n_1}, \frac{1}{n_2} \text{ and } \frac{1}{n_3}$$

$\Rightarrow$ 1, 1 and 1

The LCM is 1, therefore

$h : k : l = 1 : 1 : 1$

Miller indices are (1 1 1)

Problem 4. **Find the density of unit cell of FCC crystal. Given edge length of the unit cell is 4.8Å and the molecular mass of the element is 54 g mole^{-1}.**

Solution :

For FCC crystal, the number of molecule per unit cell is 4. The moleculer mass of the element = 54 g mole^{-1}, The Avogagdro's number N = 6×10^{23} per gm.

Now, density of unit cell $= \frac{4M}{Na^3}$

$$= \frac{4 \times 54}{6 \times 10^{23} \times (4.8 \times 10^{-8})^3}$$

$$= \frac{216}{3185} \times 10$$

$$= 0.678 \text{ gm per cc}$$

Problem 5. **The density of α-iron is 7080 kg m^{-3} and its atomic weight is 56. Given that α-iron crystallises in BCC space lattice (i) find the lattice parameter and (ii) the bond length *i.e.* the distance between the nearest atoms. Given Avogadro's number is 6.02×10^{26} kg^{-1}.**

Solution :

We know that density

$$\rho = \frac{nA}{VN}$$

where V is the volume, $V = a^3$

Hence $$\rho = \frac{nA}{a^3 N}$$

or $$a^3 = \frac{nA}{N\rho}$$

$$= \frac{2 \times 56}{6.02 \times 10^{26} \times 7080}$$

$$a^3 = 0.000262 \times 10^{-27}$$

$$a = (.000262 \times 10^{-27})^{1/3}$$

$$= 0.137 \times 10^{-9} \text{ m}$$

Bond length $$= 2r$$

$$= 2 \frac{\sqrt{3}}{4} a$$

$$= 2 \times \frac{\sqrt{3}}{4} \times 0.137 \times 10^{-9}$$

$$= 0.118 \times 10^{-9} \text{ m}$$

Problem 6. **An element having BCC structure has atomic mass 50. Calculate the density of the unit cell if its edge length is 176 picometre.**

Solution :

edge length, $a = 176 \times 10^{-12}$ m

For BCC, number of atoms in unit cell, $z = 2$

Atomic mass of the element M = 50 g mole^{-1}

$= 50 \times 10^{-3}$ kg mole^{-1}

Avogadro's number = 6.02×10^{26} per kg.

Now, density $\rho = \frac{ZM}{a^3 N}$

$$= \frac{2 \times 50}{(176 \times 10^{-12})^3 \times (6.02 \times 10^{26})}$$

$$= 304.69 \times 10^3 \text{ kg m}^{-3}$$

Problem 7. **Lattice constant of a cubic lattice is 2.82 Å. Determine the spacing between two successive parallel planes of a family of planes $(h\ k\ l)$ having Miller indices as (121), (101) and (001) planes.**

Solution :

Here $a = 2.82$ Å

Now the separation or spacing d between two successive parallel planes of a family of planes $(h\ k\ l)$ in a cubic system is given as

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

(i) For (121) plane

$$h = 1,\ k = 2 \text{ and } l = 1$$

$$\therefore \quad d_{121} = \frac{2.82}{\sqrt{(1)^2 + (2)^2 + (1)^2}}$$

$$= \frac{2.82}{\sqrt{6}} = \frac{2.82}{1.81}$$

$$= 1.55 \text{ Å}$$

(ii) For (101) plane

$$h = 1,\ k = 0 \text{ and } l = 1$$

$$\therefore \quad d_{101} = \frac{2.82}{\sqrt{(1)^2 + 0 + (1)^2}}$$

$$= \frac{2.82}{1.41} = 2 \text{ Å}$$

(iii) For (001) plane

$$h = 0,\ k = 0 \text{ and } l = 1$$

$$\therefore \quad d_{001} = \frac{2.82}{\sqrt{(0)^2 + (0)^2 + (1)^2}}$$

$$= 2.82 \text{ Å}$$

Problem 8. **The spacing between successive (100) planes in sodium chloride is 1.41 Å. X-rays incident on the surface of the crystal is found to give rise to second order Bragg reflections at glancing angle 10°. Calculate the wavelength of X-ray radiations.**

Solution :

Here $d = 1.41 \times 10^{-10}$ m

$\theta = 10°$

$n = 2$

$\lambda = ?$

Using the relation

$$2d \sin\theta = n\lambda$$

or $$\lambda = \frac{2d\sin\theta}{n}$$

$$= \frac{2\times1.41\times10^{-10}\times\sin10^{\circ}}{2}$$

$$= \frac{2\times1.41\times10^{-10}\times0.173}{2}$$

$$= 0.243 \text{ Å}$$

Problem 9. **The primitive translation vectors of the hexagonal space lattice are**

$$\vec{a} = \hat{i}$$

$$\vec{b} = 2\hat{i} + \hat{j}$$

$$\vec{c} = \hat{i} + \hat{k}$$

Find (i) the volume of the primitive cell of direct lattice.

(ii) primitive translation of the reciprocal lattice.

Solution :

(i) Volume V of primitive cell is given by

$$V = |\vec{a}.(\vec{b}\times\vec{c})|$$

$$= |\hat{i}.(2\hat{i}+\hat{j})\times(\hat{i}+\hat{k})|$$

$$= |\hat{i}.(2(\hat{i}\times\hat{i})+2(\hat{i}\times\hat{k})+(\hat{j}\times\hat{i})+(\hat{j}\times\hat{k}))|$$

$$= |\hat{i}.(0+2(-\hat{j})+(-\hat{k})+\hat{i})|$$

$$= |\hat{i}.(-2\hat{j}-\hat{k}+\hat{i})|$$

$$= |-2(\hat{i}.\hat{j})-\hat{i}.\hat{k}+\hat{i}.\hat{i}|$$

$$= |0-0+1|$$

$$= 1$$

(ii) The primitive translation of reciprocal lattice are

$$\vec{A} = \frac{2\pi}{V}(\vec{b}\times\vec{c})$$

$$= \frac{2\pi}{V} [(2\hat{i} + \hat{j}) \times (\hat{i} + \hat{k})]$$

$$= \frac{2\pi}{V} [-2\hat{j} - \hat{k} + \hat{i}]$$

Putting $V = 1$, we get

$$\vec{A} = 2\pi (\hat{i} - 2\hat{j} - \hat{k})$$

$$\vec{C} = \frac{2\pi}{V} (\vec{a} \times \vec{b})$$

$$= \frac{2\pi}{V} [\hat{i} \times (2\hat{i} + \hat{j})]$$

$$= \frac{2\pi}{V} [2(\hat{i} \times \hat{i}) + (\hat{i} \times \hat{j})]$$

$$= 2\pi [0 + \hat{k}] \qquad [\because V = 1]$$

$$= 2\pi \hat{k}$$

$$\vec{B} = \frac{2\pi}{V} (\vec{c} \times \vec{a})$$

$$= \frac{2\pi}{V} ((\hat{i} + \hat{k}) \times \hat{i})$$

$$= \frac{2\pi}{V} [(\hat{i} \times \hat{i}) + (\hat{k} \times \hat{i})]$$

$$= 2\pi [0 + \hat{j}]$$

$$= 2\pi \hat{j}$$

Problem 10. **X-rays of wavelength 1.01 Å make a glancing angle of 8° in the first order when diffracted from NaCl crystal. Find the lattice constant of NaCl.**

Solution :

Here, $\lambda = 1.01 \times 10^{-10}$ m

$n = 1$

$\theta = 8°$

$\sin 8° = 0.1391$

Using the relation, $2d \sin\theta = n\lambda$ we have

$$d = \frac{n\lambda}{2\sin\theta}$$

$$= \frac{1\times1.01\times10^{-10}}{2\times0.1391}$$

$$= 3.63 \text{ Å}$$

Problem 11. **If X-rays of wavelength 1.5 Å are diffracted at an angle of 10° in the first order, what is the spacing between the adjacent planes of the crystal ? At what angle will second order maximum occur ?**

Solution :

Here $\lambda = 1.5 \times 10^{-10}$ m

$\theta = 10°$

$\sin 10° = 0.1736$

$n = 1$

Using Bragg's law, $2d \sin\theta = n\lambda$, we have

$$d = \frac{n\lambda}{2\sin\theta}$$

$$= \frac{1.5\times10^{-10}}{2\times0.1736} = 4.32 \times 10^{-10} \text{ m}$$

For second order maximum, let θ' be the angle of Bragg reflection then,

$$2d \sin\theta' = n\lambda$$

or $$\sin\theta' = \frac{n\lambda}{2d}$$

$$= \frac{2\times1.5\times10^{-10}}{2\times8.64\times10^{-10}}$$

$$= 0.1736$$

$$\theta = \sin^{-1}(0.1736)$$

$$= 20° 1'$$

Problem 12. **The primitive translation vectors of the hexagonal space lattice are**

$$\vec{a} = \left(\frac{a}{2}\right)\hat{i} + \left(\frac{a}{16}\right)\hat{j}$$

$$\vec{b} = \frac{-a}{2}\hat{i} + \left(\frac{a}{16}\right)\hat{j}$$

$$\vec{c} = c\,\hat{k}$$

Find (i) volume of primitive cell (ii) primitive translation of the reciprocal lattice.

Solution :

Volume of the primitive cell is given by

$$V = \vec{a} \cdot (\vec{b} \times \vec{c})$$

$$= \left(\frac{a}{2}\hat{i} + \frac{a}{16}\hat{j}\right) \cdot \left(-\frac{a}{2}\hat{i} + \frac{a}{16}\hat{j}\right) \times c\,\hat{k}$$

$$= \left(\frac{a}{2}\hat{i} + \frac{a}{16}\hat{j}\right) \cdot \left[-\frac{ac}{2}(\hat{i} \times \hat{k}) + \frac{ac}{16}(\hat{j} \times \hat{k})\right]$$

$$= \left(\frac{a}{2}\hat{i} + \frac{a}{16}\hat{j}\right) \cdot \left[\frac{ac}{2}\hat{j} + \frac{ac}{16}\hat{i}\right]$$

$$= \frac{a^2 c}{32}(\hat{i} \cdot \hat{i}) + \frac{a^2 c}{32}(\hat{j} \cdot \hat{j})$$

$$= \frac{a^2 c}{32} + \frac{a^2 c}{32} = \frac{a^2 c}{16}$$

Let the primitive translation of reciprocal lattice be $\vec{A}$, $\vec{B}$ and $\vec{C}$, then

$$\vec{A} = 2\pi \frac{\vec{b} \times \vec{c}}{V}$$

$$= \frac{32\pi}{a^2 c}\left[\left(-\frac{a}{2}\hat{i} + \frac{a}{16}\hat{j}\right) \times c\hat{k}\right]$$

$$= \frac{32\pi}{a^2 c}\left[\frac{ac}{2}\hat{j} + \frac{ac}{16}\hat{j}\right]$$

$$\vec{A} = \frac{16\pi}{a}\hat{j} + \frac{2\pi}{a}\hat{i}$$

$$= \frac{2\pi}{a}\hat{i} + \frac{16}{a}\hat{j}$$

$$\vec{B} = 2\pi \frac{\vec{c} \times \vec{a}}{V}$$

$$= \frac{2\pi \times 16}{a^2 c}\left[c\hat{k} \times \left(\frac{a}{2}\hat{i} + \frac{a}{16}\hat{j}\right)\right]$$

$$= \frac{32\pi}{a^2 c}\left[\frac{ac}{2}\hat{j} - \frac{ac}{16}\hat{i}\right]$$

$$= \frac{-2\pi}{a}\hat{i} + \frac{16\pi}{a}\hat{j}$$

$$\vec{C} = 2\pi \frac{\vec{a} \times \vec{b}}{V}$$

$$= \frac{32\pi}{a^2 c}\left[\left(-\frac{a}{2}\hat{i} + \frac{a}{16}\hat{j}\right) \times \left(\frac{-a}{2}\hat{i} + \frac{a}{16}\hat{j}\right)\right]$$

$$= \frac{32\pi}{a^2 c}\left[\frac{a^2}{32}\hat{k} + \frac{a^2}{32}\hat{k}\right]$$

$$= \frac{32\pi}{a^2 c}\left[\frac{a^2}{16}\hat{k}\right]$$

$$= \frac{2\pi}{c}\hat{k}$$

CONCEPTUAL QUESTIONS

Q. 1. **Why are most solids crystalline in nature ?**

Ans. Crystalline form of solid has a low energy state. The energy released during the formation of an ordered crystal is more than that released during the formation of the disordered crystal. Thus due to low energy state, most solids are crystalline in nature.

Q. 2. **What is a primitive cell ?**

Ans. A primitive cell is a type of unit cell which contains only one lattice point at corners and is a minimum volume unit cell.

Q. 3. **Determine the number of nearest neighbour for mono atomic SC and BCC structures.**

Ans. For SC crystal, the number of nearest neighbours is 6 with coordinates (100), $(\bar{1}00)$, (010), $(0\bar{1}0)$, (001) and $(00\bar{1})$ and for BCC the number of nearest neighbours is 8

with coordinates $\left(\frac{1}{2}\frac{1}{2}\frac{1}{2}\right)$, $\left(\frac{1}{2}\frac{\bar{1}}{2}\frac{\bar{1}}{2}\right)$, $\left(\frac{1}{2}\frac{\bar{1}}{2}\frac{1}{2}\right)$, $\left(\frac{\bar{1}}{2}\frac{\bar{1}}{2}\frac{1}{2}\right)$, $\left(\frac{\bar{1}}{2}\frac{\bar{1}}{2}\frac{\bar{1}}{2}\right)$, $\left(\frac{\bar{1}}{2}\frac{1}{2}\frac{1}{2}\right)$ and $\left(\frac{\bar{1}}{2}\frac{1}{2}\frac{\bar{1}}{2}\right)$.

Q. 4. Does 5 fold symmetric axis exist in lattice ? Explain.

Ans. No, five fold symmetric axis does not exist in lattice. If the lattice has 5 fold symmetry then the unit cell of the lattice will be pentagon. As by definition, the unit cell fill entire space by translational operator, so it is not possible to fill the entire space and hence five fold symmetry is not possible.

Q. 5. What is a translation operation ?

Ans. A translation operation is a kind of symmetry operation which when performed leaves the crystal invariant.

Q. 6. What do your mean by a space group ? Give its physical significance.

Ans. The group of all the symmetry elements of a crystal structure is called space group. It determines the symmetry of the crystal structure as a whole.

Q. 7. Can a face centered tetragonal space lattice exist ? Explain.

Ans. No. Two face centered tetragonal lattices ABCD and CDEF are placed side by side in Fig. 1.69.

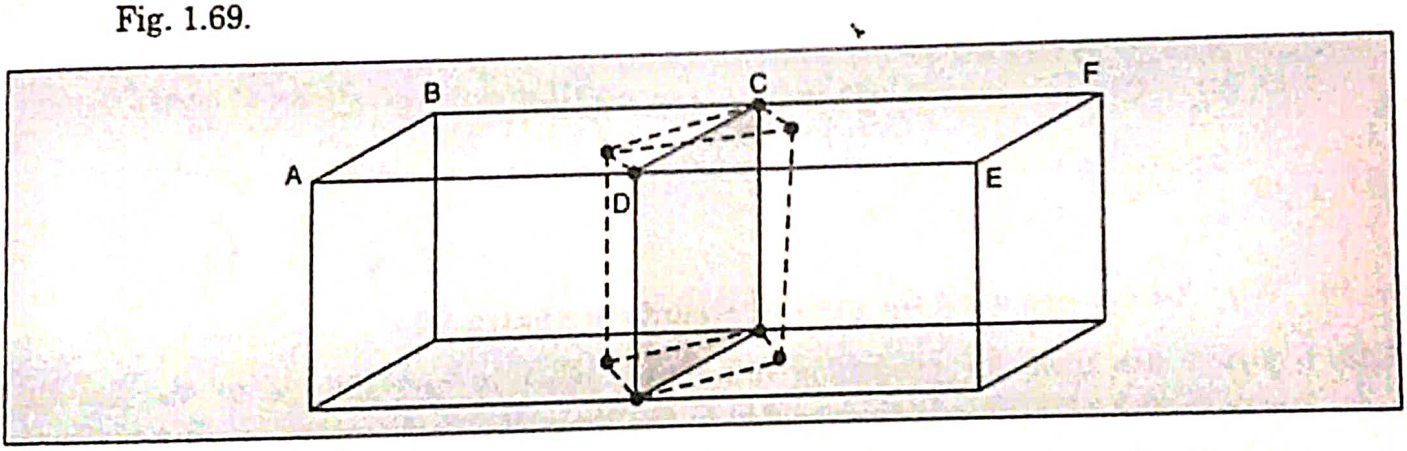


Fig. 1.69.

The dotted lines shown in Fig. 1.69 produce a body centered tetragonal space lattices. Hence a face centered tetragonal space lattices in a crystal lying side by side merge into a body centered space lattice and so there cannot be any face centered tetragonal space lattice.

Q. 8. How many atoms are there in the primitive cell of a diamond ? What is the length of a primitive translation vector if the cube edge length is 3.5 Å.

Ans. Diamond has FCC Bravais lattice with two carbon atoms in a primitive cell. The number of atoms in a cube is 8. If $\vec{a}$ is the cube edge length, then,

Primitive translation vector = $\frac{a}{\sqrt{2}}$

$$= \frac{3.5}{1.41} = 2.48 \text{ Å}$$

Q. 9. Find the ratio of the number of particles in planar (110) and (111) in case of simple cubic structure.

Ans. Let d be the separation between plane $(h\ k\ l)$ and δ be the particle density per unit area in plane $(h\ k\ l)$

For (100) plane, $d = \frac{a}{\sqrt{2}}$ and $\delta = \frac{n_1}{a^2\sqrt{2}}$

For (111) plane, $d = \frac{a}{\sqrt{3}}$ and $\delta = \frac{n_2}{\frac{\sqrt{3}}{2}a^2}$

Hence $\frac{\frac{a\sqrt{2}}{n_1}}{\frac{a^2\sqrt{2}}{\frac{a}{\sqrt{3}}}}$ gives $n_1 = 2n_2$

$$\frac{\frac{n_2}{\frac{\sqrt{3}}{2}a^2}}{}$$

or $\frac{n_1}{n_2} = 2$

Q. 10. Why X-rays are used for crystal structure analysis ?

Ans. X-rays are used for producing diffraction effect in crystals due to the fact that wavelength of X-rays is comparable to the inter atomic distances in actual crystals. For example, X-rays produced by a acceleration of electrons through a potential difference of 19kV gives wavelength λ as

$$\lambda = \frac{hc}{eV}$$

$$= \frac{6.62\times10^{-34}\times3\times10^{8}}{1.6\times10^{-19}\times10^{4}}$$

$$= 1.24 \text{ Å}$$

This wavelength of 1.24 Å is very close to the interatomic spacing of an actual crystal. In NaCl crystal, the interatomic spacing is 2.8 A°. Only X-rays are scattered elastically without change of wavelength by the charged particles of the atom.

Q. 11. How does Bragg's reflection differ from ordinary reflection ?

Ans. The phenomenon of Bragg's reflection is similar to the diffraction of light whereas in ordinary reflection all the reflected waves are in phase and there are no maxima and minima. In Bragg's reflection various parallel planes of the crystal serve the same purpose as the ruled lines on the grating which produce opacities and transparencies.

Q. 12. What is K-space ?

Ans. The reciprocal lattice points in three dimensional space form a reciprocal lattice space. This reciprocal lattice space is called K-space. The coordinates of points in this space are defined by (h k l), the Miller indices.

Q. 13. What are the uses of Laue's diffraction pattern ?

Ans. Laue's diffraction pattern are used in

(i) determining the microscopic structure of crystals for the study of mechanical processes of rolling, hardening and annealing.

(ii) locating as well as determining angular relationship between different planes in crystal lattice which are rich in atoms.

Q. 14. Why reciprocal lattice is so named ?

Ans. Because the length assigned to each normal representing the reciprocal lattice is proportional to the reciprocal of the interplaner spacing of that plane in ordinary space.

Q. 15. What is the diffraction condition in terms of reciprocal lattice vector $\vec{G}$?

Ans. The diffraction condition in terms of reciptocal lattice vector $\vec{G}$ is given by

$$2\,\vec{K}\,.\,\vec{G} + G^2 = 0$$

or
$$2\,\vec{K}\,.\,\vec{G} = -G^2$$

where K is the wave vector for an X-rays and is given by $\vec{K} = K_x\,\hat{i} + K_y\,\hat{j} + K_z\,\hat{k}$

and
$$\vec{G} = h\,\vec{A} + k\,\vec{B} + l\,\vec{C}$$

Q. 16. Calculate the spacing between adjacent lattice planes of a crystal in terms of reciprocal space lattice.

Ans. Let the reciprocal lattice G be given by

$$\vec{G} = h'\vec{A} + k'\vec{B} + l'\vec{C}$$

Let $\hat{n}$ be unit vector normal to the (h k l) plane of the direct lattice. As the reciproca lattice is perpendicular to the direct lattice

$$\hat{n} = \frac{\vec{G}}{|G|}$$

If $\vec{a}$, $\vec{b}$ and $\vec{c}$ are the primitive translation vectors, then the spacing d is given by

$$d = \frac{\vec{a}.\hat{n}}{h}$$

$$= \frac{\vec{a}.\vec{G}}{hG}$$

$$= \frac{\vec{a}.(h'\vec{A}+k'\vec{B}+l'\vec{C}}{hG}$$

$$= \frac{2\pi}{G}\frac{h'}{h}$$

$$= \frac{2\pi n}{G}$$

Because $n = \frac{h'}{h}$ and $\vec{a} \cdot \vec{A} = 2\pi$, $\vec{a} \cdot \vec{B} = 0$ and $\vec{a} \cdot \vec{C} = 0$

Q. 17. Name two methods to derive the conditions of diffraction in crystals.

Ans. Two methods to derive the conditions of diffraction in crystals are

(i) due to Bragg

and (ii) due to Von Laue

Q. 18. When does the Bragg's law not operative ?

Ans. The Bragg's law is a consequence of the periodicity of the crystal lattice. The law is not operative in terms of the arrangement of atoms in the basis. From Bragg's law, we obtain diffraction only when $\lambda \leq 2d$, otherwise it is not operative. Thus, with long wavelength the law does not operate and we cannot obtain Bragg reflection with visible light.

Q. 19. Prove that every reciprocal lattice vector is normal to lattice plane of crystal lattice.

Ans. Let the reciprocal translation reciprocal vector G be given a

$$G = h'\vec{A} + k'\vec{B} + l'\vec{C}$$

Consider a plane $(h\ k\ l)$, the intercepts of the plane are $\left(g\frac{a}{h}, g\frac{b}{k}, g\frac{c}{l}\right)$ = $(n_1 a, n_2 b, n_3 c)$

Hence the vectors $n_2(\vec{b} - n_1\vec{a})$, $(n_3\vec{c} - n_2\vec{b})$ and $(n_1\vec{a} - n_3\vec{c})$ lies in the plane $(h\,k\,l)$

If $\vec{G'}$ is perpendicular to the plane $(h\ k\ l)$ then

$$n_2(\vec{b} - n_1\vec{a}) \cdot \vec{G'} = 0$$

$$(n_3\vec{c} - n_2\vec{b})\ \vec{G'} = 0$$

$$(n_1\vec{a} - n_3\vec{c}) \cdot \vec{G'} = 0$$

or $$n_2 k' - n_1 h' = 0$$

$$n_3 l' - n_2 k' = 0$$

and $$n_1 h' - n_3 l' = 0$$

From above equations, we get

$$n_1 h' = n_2 k' = n_3 l' = \text{constant}$$

or $$\frac{g}{h} h' = \frac{g}{k} k' = \frac{g}{l} = \text{constant}$$

or $$h' = z h,\ k' = z k \text{ and } l' = z l$$

Therefore the vector normal to the plane $(h\ k\ l)$ is

$$\vec{G'} = h'\vec{A} + k'\vec{B} + l'\vec{C} = z\ (h\vec{A} + k\vec{B} + l\vec{C})$$

$$= z\,G$$

As $$\vec{G'} = z\ \vec{G}$$

Hence $\vec{G'}$ is parallel to $\vec{G}$

Thus, $\vec{G}$ is normal to plane $(h\ k\ l)$

Thus, we can say that $\vec{G} = (h\vec{A} + k\vec{B} + l\vec{C})$ is normal to the plane $(h\ k\ l)$

Q. 20. What is Ewald's construction ?

Ans. Ewald's construction is the geometric representation of diffraction condition. From Laue's condition of diffraction, we have

$$D\vec{k'} = \vec{G}$$

where $\vec{G}$ is the reciprocal lattice vector.

When a beam of X-ray is incident on the plane $(h\ k\ l)$ the diffraction condition is

$$\Delta\ \vec{k} = \vec{k'} - \vec{k}$$

$$= \vec{G}$$

or $$\vec{k'} = \vec{k} + \vec{G}$$

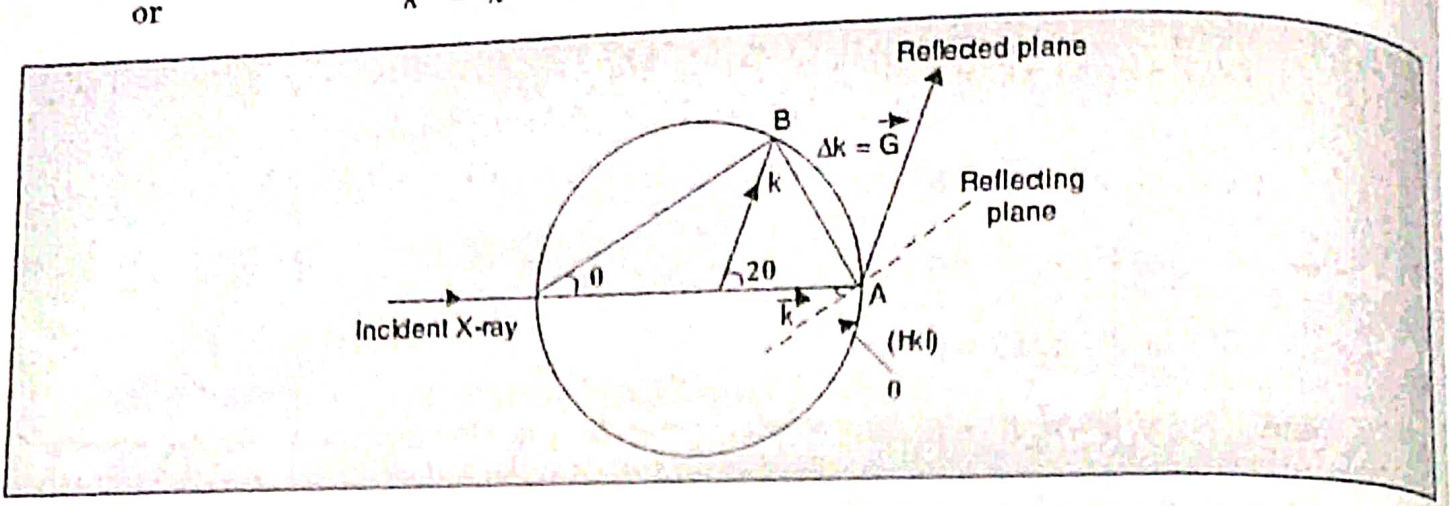


Fig. 1.70.

Also we know that,

$$|\vec{k'}| = |\vec{k}| = \frac{2\pi}{\lambda}$$

In the Ewald construction shown in Fig. 1.70, the sphere does not intersect any other point in the reciprocal lattice. Hence X-ray will be unable to diffract when incident at angle θ.

As $$\vec{k'} = \vec{k} + G$$

$$k'^2 = k^2 + G^2 + 2k \cdot G$$

For elastic scattering

$$k'^2 = k$$

$$\therefore \quad \overrightarrow{G^2} + 2\vec{k} \cdot \vec{G} = 0$$

or $$2\vec{k} \cdot \vec{G} = |G|^2$$

This is another statement of Bragg's law.

Q. 21. Mention some important features of Miller indices ?

Ans. (i) Parallel planes having equal space possess same index numbers.

(ii) A plane passing through its origin is defined in terms of a parallel plane having non-zero intercept.

(iii) If a plane is parallel to the coordinate axis then the intercept of this plane is infinity and hence its Miller index is zero.

(iv) Ratio of indices is more important as it determines a plane. For example (2 4 6) and (1 2 3) represent the same plane.

(v) The direction (h k l) is perpendicular to the plane (h k l).

Q. 22. Why do we take reciprocals to find Miller indices ?

Ans. We take reciprocals to find Miller indices so as to bring all the plans inside a single unit cell. As the whole crystal can be produced from a single unit cell, the unit cell is considered as a representative of the entire crystal. Thus the study of unit cell gives the characteristics of the whole crystal.

Q. 23. Draw the plane (100) and (010).

Ans. (i) (100) plane lies in the y-z-plane and has an intercept 1 along the X-axis as shown in Fig. 1.71.

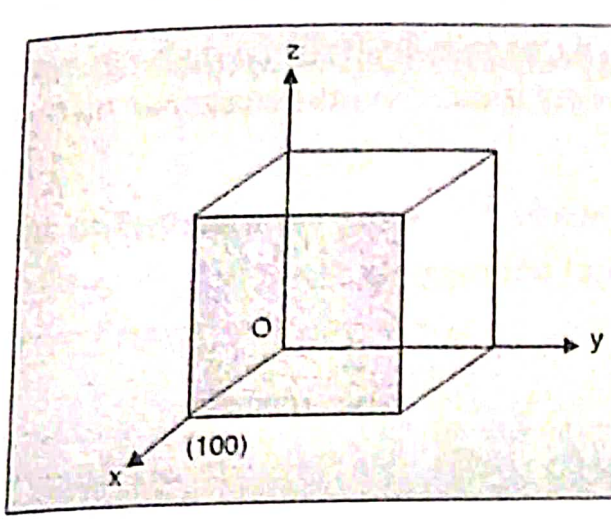


Fig. 1.71.

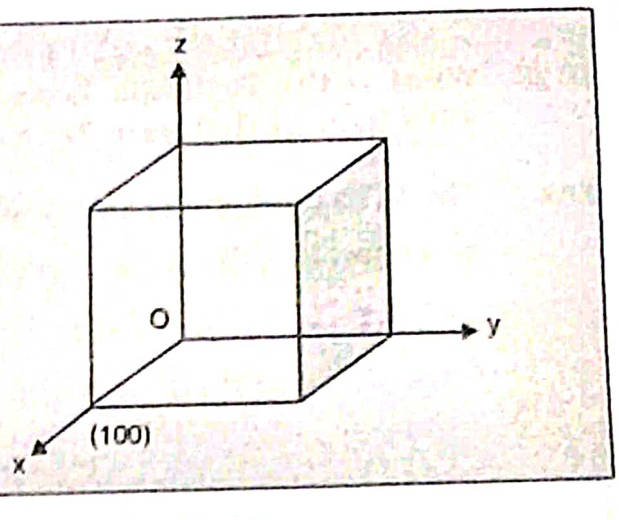


Fig. 1.72.

(ii) (010) plane lies in the x-z plane and has an intercept 1 along the y-axis as shown in Fig. 1.72.

Q. 24. Explain the meaning of (322) and (111) planes.

Ans. (322) plane has Miller indices 3, 2, 2. Its intercepts on $\vec{a}$, $\vec{b}$ and $\vec{c}$ axes are $\frac{1}{3}$, $\frac{1}{2}$ and $\frac{1}{2}$. Taking the whole numbers, the intercepts are 2, 3, 3 *i.e.* $2a$, $3b$ and $3c$.

Similarly (111) plane has Miller indices. Its intercepts on $\vec{a}$, $\vec{b}$ and $\vec{c}$ axes are 1, 1 and 1 *i.e.* $\vec{a}$, $\vec{b}$ and $\vec{c}$.

Q. 25. Calculate the separation between lattice planes in a face centered (FCC) structure.

Ans. In FCC lattice there is one unit situated at each corner and one unit at the centre of each of the six faces. Thus an additional (100) plane arises half way between the (100) planes. These additional planes pass through the centre of the front and back face. As the distance between (100) planes of a simple cubic lattice is a, the distance between (100) plane of the FCC lattice is $\frac{a}{2}$.

$$\therefore \qquad d_{100} = \frac{1}{2}\, a$$

Similarly, an additional set of (110) planes parallel to the first set arises midway between the planes of simple cubic lattice.

$$\therefore \qquad d_{110} = \frac{1}{2}\left(\frac{a}{\sqrt{2}}\right)$$

The (111) planes of simple cubic lattice pass through the centre of all the faces of FCC lattice and hence no new planes arise in this case.

$$\therefore \qquad d_{111} = \frac{a}{\sqrt{3}}$$

Q. 26. What is the Brillouin Zone and draw a two dimensional hexagonal lattice with its first Brillouin Zone?

Ans. The Brillouin Zone is the ensemble of independent $\vec{K}$-vectors not connected to any $\vec{G}$-vector. It is the primitive cell of the reciprocal lattice vector.

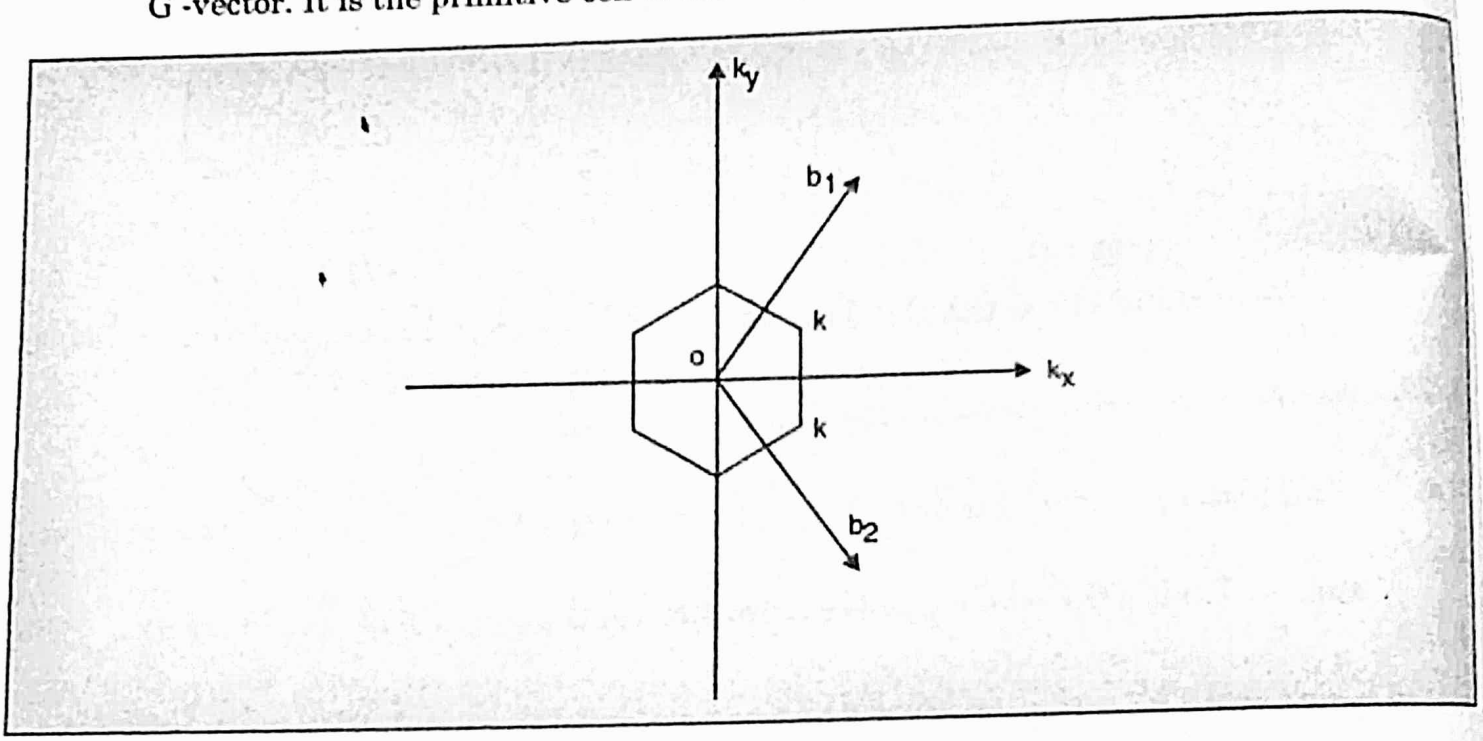


Fig. 1.73.

Fig. 1.73 represents a first Brillouin Zone with O as the zone-center and K is at the corner.

Q. 27. What do you mean by a Bragg plane ?

Ans. Bragg plane is a plane in reciprocal space which bisects a reciprocal lattice vector $\vec{k}$ at right angles and is defined as a part of Von Laue condition for diffraction peaks in X-ray diffraction crystallography. Here $\vec{k}$ is the wave vector given by

$$\vec{k} = \frac{2\pi}{\lambda}\hat{n}$$

Q. 28. What are Bravais lattices ?

Ans. In three dimensions there are only 14 ways of arranging points in space to make a lattice which satisfy $T = r + n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$ and having certain number of symmetry operations. These 14 lattices are referred as Bravais lattices.

MULTIPLE CHOICE QUESTIONS

Choose the correct alternative for each question given below :

1. **Sodium metal crystallizes in body centered cubic lattice with cell edge 4.29 Å. The radius of the sodium atom is**

   (a) 1.76 Å (b) 1.86 Å

   (c) 0.86 Å (d) 0.76 Å

2. **The Miller indices of a plane in a lattice**

   (a) are the coordinates of the shortest reciprocal lattice vector normal to the plane.

   (b) do not depend on the particular choice of primitive vector.

   (c) cannot be defined for hexagonal crystal lattices.

   (d) are proportional to the intercepts of that plane with the crystal axes.

3. **The unit cell with dimensions $\alpha = \beta = \gamma = 90$, $a = b \neq c$ is**

   (a) cubic (b) triclinic

   (c) hexagonal (d) tetragonal

4. **Total volume of atoms present in FCC unit cell of metal in terms of radius of an atom is**

   (a) $\frac{24}{3}\pi r^3$ (b) $\frac{12}{3}\pi r^3$

   (c) $\frac{16}{3}\pi r^3$ (d) $\frac{20}{3}\pi r^3$

5. **BCC lattice is reciprocal lattice of**

   (a) SC lattice (b) FCC lattice

   (c) BCC lattice (d) Hexagonal lattice

6. **Chromium has BCC structure. Its atomic radius is 0.1249 nm. The free volume per unit cell is**

   (a) 0.00767 $(nm)^3$ (b) 0.0767 $(nm)^3$

   (c) 0.024 $(nm)^3$ (d) 0.0024 $(nm)^3$

7. **The study of geometric form and other physical properties of crystalline solids by using X-rays, electron beam and neutron beam constitute.**

(a) spectroscopy (b) physiotherapy

(c) crystallography (d) none

8. **The number of Bravais lattice in three dimensions is**

(a) 256 (b) 14

(c) 37 (d) 07

9. **The total number of atoms per unit cell of diamond is**

(a) 2 (b) 4

(c) 6 (d) 8

10. **If the number of lattice points per unit cell is one, then it is called ..... unit cell.**

(a) primitive (b) non-primitive

(c) both a and b (d) non

11. **The first Brillouin Zone of FCC lattice is**

(a) simple cubic (b) Rhombic dodecahedron

(c) truncated octahedron (d) none

12. **The Miller indices for octahedral plane in cubic crystal**

(a) (100) (b) (110)

(c) (111) (d) none

13. **Another name for lattice points is**

(a) lattice sites (b) lattice arrangements

(c) lattice circles (d) lattice array

14. **Which type of radiations are used to study the structure of crystals.**

(a) visible light (b) X-rays

(c) γ-rays (d) u-v-rays

15. **Topaz, an orthorhombic semiprecious stone, has a ratio of lattice parameters $a : b : c$ of 0.529 : 1.0 : .477. Find the Miller indices of the face whose intercepts are as follows (0.264; : 1.0; 0.238)**

(a) (2 1 2) (b) (1 2 2)

(c) (2 2 1) (d) (2 2 2)

16. **X-rays with a wavelength of 0.58 A° are used for calculating d_{200} in nickel. The Bragg's reflection angle is 9.5 what is lattice parameter a ?**

(a) 3.155 Å (b) 3.515 Å

(c) 3.551 Å (d) 3215 Å

17. **How many carbon atoms are there in a unit cell of diamond ?**

(a) 10 (b) 8

(c) 6 (d) 4

18. Which one of the following metals is truly isotropic ?

(a) iron (b) aluminium

(c) copper (d) tungsten

19. Bragg's law in terms of reciprocal lattice vector G is

(a) $2K.G + K^2 = 0$ (b) $2K.G + G^2 = 0$

(c) $G.G + 2K.2K = 0$ (d) $2G \, . \, G + K.K = 0$

20. The reciprocal lattice for hexagonal space lattice is

(a) BCC lattice (b) HCP

(c) FCC lattice (d) SCC

21. If a is lattice constant and λ the wavelength of the X-rays then for no diffraction to occur the condition is

(a) $a < \lambda < 2a$ (b) $\lambda < a$

(c) $\lambda >$ (d) $\lambda > 2a$

22. A crystal reflects monochromatic X-rays strongly when the Bragg's glancing angle for the first order reflection is 30°. The glancing angle for the second order is

(a) 45° (b) 60°

(c) 75° (d) 90°

23. The Miller indices of the plane parallel to the X and Y axes are

(a) (100) (b) (010)

(c) (001) (d) (111)

24. In case of FCC crystal with Z atoms of A-type and 2 atoms of B-type, $(h'k'l')$ reflection has intensity

(a) Maximum when all are odd or even

(b) Maximum only when all are even

(c) Maximum only when all are odd

(d) It is maximum or minimum depends on which type of atom occupies specific position.

Answers

1.	(b)	2.	(a)	3.	(d)	4.	(c)	5.	(b)
6.	(a)	7.	(c)	8.	(b)	9.	(d)	10.	(a)
11.	(c)	12.	(c)	13.	(a)	14.	(b)	15.	(a)
16.	(b)	17.	(b)	18.	(d)	19.	(b)	20.	(b)
21.	(d)	22.	(d)	23.	(c)	24.	(a)		

HINTS/SOLUTIONS

1. $r = \frac{\sqrt{3}}{4} a$

$$= \frac{1.732 \times 4.29}{4} = 1.81 \text{ Å}$$

4. No. of atoms present in FCC unit cell = 4

Total volume of atoms present in FCC unit cell,

$$V = 4x \frac{4}{3} \pi \lambda^3$$

$$= \frac{16}{3} \pi \lambda^3$$

6. Given $r = 0.1249$ nm

$$a = \frac{4}{\sqrt{3}} r = \frac{4}{\sqrt{3}} \times 0.1249$$

$$= 0.28845 \text{ nm}$$

Volume of unit cell, $V = a^3 = (0.28845)^3$

$$= 0.024 \text{ nm}^3$$

Number of atoms in BCC unit cell = 2

Hence volume per unit cell $(v) = \frac{4}{3} \pi r^3 \times 2$

$$= 0.01633 \text{ (nm)}^3$$

Free volume per unit cell $\Delta V = V - v$

$$= 0.00767 \text{ (nm)}^3$$

15. Miller indices of the plane are

$$\left(\frac{0.529}{0.264} \quad \frac{1.0}{1.0} \quad \frac{0.477}{0.238} \right)$$

or (2 1 2)

16. $d_{200} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$

$$= \frac{a}{\sqrt{(2)^2 + 0 + 0}} = \frac{a}{2}$$

Using Bragg's law, we have

$2d \sin\theta = n\lambda$

$$2 \times \left(\frac{a}{2}\right) \times \sin 9.5° = 1 \times \lambda$$

or $$\vec{a} = \frac{0.58\,A°}{0.165} = 3.515\,A°$$

CHAPTER AT A GLANCE

1. **A solid** is a material, distinguished for its constancy of form and volume and are classified as crystalline and amorphous.
2. **Crystals** are solids which have a regular periodic arrangement of particles. They can be mono or poly crystals.
3. **A crystal lattice** is an array of points related by the lattice translation operator, T $= n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c}$ where n_1, n_2 and n_3 are integers and $\vec{a}$, $\vec{b}$ and $\vec{c}$ are the translation vectors. Crystal lattice is also called space lattice.
4. **Basis** is defined by the way of filling up of points of space lattice by atoms. The unit assembly of atoms located at each lattic point is called a basis.
5. **Unit cell** is produced by a space lattice combined with a basis. A unit cell is the basic building block in the crystal structure.
6. **Bravais lattice** is the set of points defined by all integral linear combinations of primitive translation vectors. There are five Bravais lattices in two dimensions and fourteen in three dimensions.
7. **Miller Indices** are used to specify the directions and planes in lattices or in crystals and are defined as the reciprocals of the intercepts of the plane on the three crystallographic axes used to specify plane in the crystal.
8. **Simple crystal structures** include the BCC, FCC, *h c p*, diamond, NaCl, CsCl, simple cubic, ZnS and hexagonal ZnS structure.
9. **A point group** is the collection of the symmetry operations excluding translations which leave a body invariant. In two dimension we have rotations and rotational reflections making a total of 10 point groups. In three dimensions these include rotations, rotational reflections and rotational inversions, making a total of 32 point groups.
10. **Space Group** is a repetitive pattern of the symmetry elements of a given crystal structure. It is the ensemble of symmetry elements that leaves the space invariant since it includes translations. There are 17 two dimensional and 230 three dimensional space groups.
11. **Reciprocal lattice** represents the diffraction pattern. A reciprocal lattice has the form

$$\vec{G} = h\vec{A} + k\vec{B} + l\vec{C}$$

12. **Bragg's law has two common forms**

(i)$2d \sin\theta = n\lambda$

(ii)$2\ \vec{K}\ .\ \vec{G} + G^2 = 0$

or$2\ \vec{K}\ .\ \vec{G} = \overrightarrow{G^2}$

13. **Von Laue's equations are**

$\vec{a}\ .\ \vec{N} = n\,h\,\lambda$

$\vec{b}\ .\ \vec{N} = n\,k\,\lambda$

and $\vec{c}\ .\ \vec{N} = n\,l\,\lambda$

14. **Brillouin Zones** correspond to primitive cells of a different type that come up in the theory of electronic levels in a periodic potential.

15. **The First Brillouin Zone** is the Wigner-Seitz primitive cell of the reciprocal lattice and in a geometric construction to the Wigner-Seitz cell in the K-space. The type of crystal lattice and corresponding first Brillouin zone are

(i)Simple cubic ..... cube

(ii)BCC ..... Rhombic dodecahedron

(iii)FCC ..... Truncated octahedron

16. **Wigner-Seitz primitive cell** is another method of choosing a cell of volume V given by a relation

$V = \vec{a}\ .\ (\vec{b} \times \vec{c})$ where $\vec{a}$, $\vec{b}$ and $\vec{c}$ are the primitive area vectors

(i)First draw lines to connect a given lattice point to all near by lattice points.

(ii)At the mid points and normal to these lines draw new lines or planes. The smallest volume enclosed in this way is a new primitive cell called Wigner-Seitz primitive cell.

17. **The atomic scattering factor** is

$$f = \int_0^{\infty} 4\pi r^2\, \rho(r) \frac{\sin Mr}{Mr}\, dr$$

18. **Total scattering amplitude**

$$F\,(h'k'l') = \sum_j e^{2\pi_j (x_j h' + y_j k' + z_j j')}$$

when all the atoms are identical

$$F\,(h'k'l') = f\xi$$

where $$\xi = \sum_j f_j \; e^{2\pi_j (x_j h' + y_j k' + z_j f')}$$

is known as geometrical structure factor.

19. **Ewald's construction** can express Bragg's law in vector form

$OA = \vec{K}$, $\overrightarrow{OB} = \vec{K'}$ and $AB = \vec{G}$ in Fig. 1.74

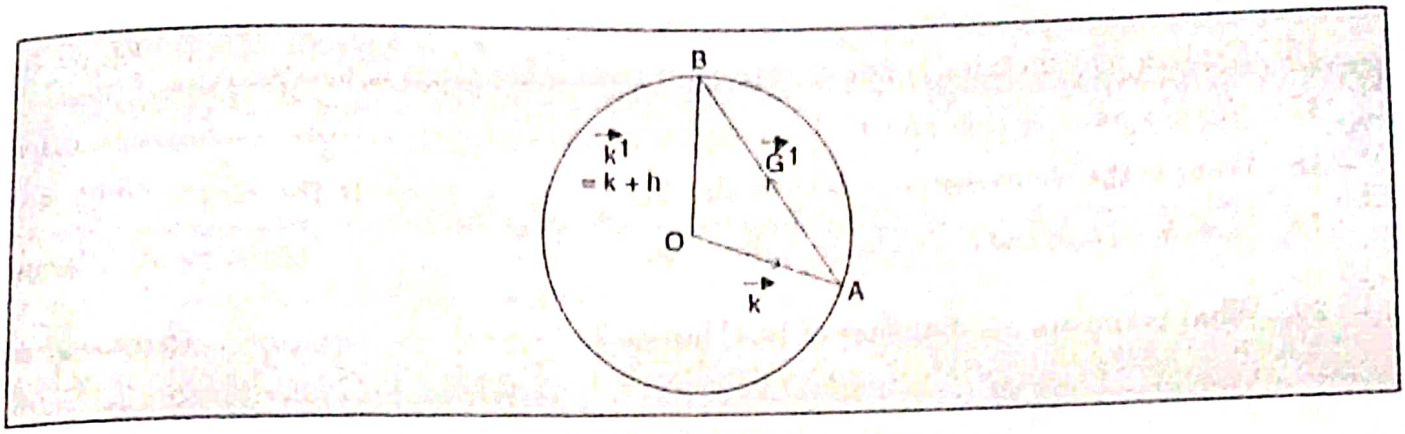


Fig. 1.74.

$$(\vec{K}+\vec{G})^2 = K^2$$

$$(\vec{K}+\vec{G})^2 = (\vec{K}+\vec{G}) \; . \; (\vec{K}+\vec{G})$$

$$= \overrightarrow{K^2}$$

or $$\overrightarrow{K^2} + \vec{G}.\vec{K} + \vec{K}.\vec{G} = \overrightarrow{K^2}$$

or $$2\,\vec{K}.\vec{G} + \overrightarrow{G^2} = 0$$

This is the main theory of elastic scattering in a periodic lattice.

SHORT ANSWER QUESTIONS

1. What is a crystal ?
2. Give the difference between crystalline and amorphous materials ?
3. Explain what do you mean by a lattice ?
4. What is a motif or basis ?
5. Define crystal structure.
6. Define a unit cell and primitive unit cell.
7. What is a condensed matter physics ?
8. What is a primitive cell and what is the volume in case of BCC and FCC lattice ?
9. Name the four types of crystalline solids ?

10. Define a metallic solid.
11. What is the meaning of word amorphous ?
12. In diamond structure what is the number of nearest neighbours?
13. What do you mean by point groups ?
14. What is a space group ?
15. Give the physical significance of packing fraction.
16. Explain why metallic bonds are stronger than other types of bonds ?
17. Name a particle that effects the material properties mostly. **(Ans.** valence electrons**)**
18. What is the mean distance between atoms. **(Ans.** In the range of 0.25 nm**)**
19. In which bond the term electron sea exist. **(Ans.** metallic bond**)**
20. What is the atomic diameter of BCC lattice ? **(Ans.** $\frac{4}{\sqrt{3}}$ a**)**
21. What are the Miller indices of octahedral plane in cubic crystal ? **[Ans.** (111)**]**
22. Define translational operators.
23. How a Wigner-Seitz cell is drawn.
24. Which type of structure NaCl possess? **(Ans.** FCC**)**
25. Why γ-rays are not used to study crystal structure?
26. What is the difference between direct lattice and reciprocal lattice?
27. What is first Brillouin Zone ?
28. Define reciprocal lattice. How is it constructed ?
29. What is the need of using reciprocal lattice ? Why should we not use direct lattice.
30. Why do crystals diffract X-rays ?
31. Define atomic scattering factor.
32. What are the considerations in deriving Laue's equations ?
33. What is the significance of Brillouin Zone ?
34. What is meant by axis of symmetry ?

LONG ANSWER QUESTIONS

1. Define space lattice, unit cell, primitive cell, basis and non primitive cell. Discuss Bravais lattice for two dimensions.
2. (a) Draw the lattice planes in simple cubic lattice.

   (b) Find an expression for spacing of planes in crystal lattices.

   (c) Discuss Bravais lattice of NaCl.

3. Explain index system for crystal planes. Draw (110), (200) and (100) planes.
4. What are Miller indices ? Derive a formula for the distance between two adjacent planes of simple cubic lattice.
5. (a) Describe the NaCl structure giving its special features.

   (b) Describe the diamond structure giving its main features.
6. Determine the inter planer spacing between two parallel planes with Miller indices $(h\ k\ l)$ of a cubic crystal of side a.
7. (a) Derive Bragg's law of crystal diffraction

   $$2d \sin\theta = n\lambda$$

   (b) Discuss briefly the methods of crystal structure determination.
8. Find the Brillouin Zone in case of

   (i) Simple cubic

   (ii) Body centered cubic lattices

   (iii) Face centered cubic lattices
9. Name the different experimental methods of X-ray diffraction by crystals. Discuss a method in detail structure analysis.
10. Explain atomic scattering factor with mathematical expression.
11. Explain geometrical structure factor with mathematical expression. How is it related to the atomic scattering factor ?
12. Define reciprocal lattice ? Derive the expression for the primitive translation vectors of the reciprocal lattice. Give the graphical representation of reciprocal lattice in two dimensions.
13. What are Laue's equations for diffraction of X-rays by a crystalline solid ? Show that these equations lead to Bragg's law for X-ray diffraction.

UNSOLVED PROBLEMS

1. The radius of copper atom which is FCC crystal is 128 Pico metre. Determine the edge length of the unit cell of copper lattice. **(Ans. 362 Pico metre)**
2. Find the Miller indices of a plane that makes an intercept at $2a$, $\frac{3}{2}b$, $1c$ on the coordinate axis of the orthogonal crystal. **(Ans. 3, 4, 6)**
3. Find the Miller indices if the given plane makes intercepts of 1, 2 and 3 Å on the crystallographic axes of a system for which the lattice parameters are in the ratio 3 : 2 : 1. **(Ans. 9 3 1)**
4. Given the density of sodium chloride unit cell as 2.21 gm/cc. If the edge length of unit cell is 5.6 Å, find the molecular mass of NaCl. **(Ans. 58.5 gm/mole)**

5. The density of an element is 7870 kg m^{-3} and its atomic mass is 55.8. Given that o iron crystallises in BCC space lattice. Find (i) the lattice parameter and (ii) the bon length *i.e.* the distance between the nearest atoms. Avogadro's number = 6.02 × 10 per kg. (Ans. 2.86 A Å, 2.48 Å)

6. An element having BCC geometry has atomic mass 50. Calculate the density of th unit cell, if its edge length is 290 × 10^{-12} m. (Ans. 6.81 × 10^{3} kg m^{-3})

7. Lattice constant of a cubic lattice is 5.64 Å. Determine the spacing between (011) (112), (101) and (100) planes. (Ans. 4 Å, 2.31 Å, 4 Å and 5.64 Å)

8. The spacing between successive (100) planes in sodium chloride crystal is 2.82 Å. X rays incident on the surface of crystal is found to give rise to first order Brag reflections at glancing angle 8.8°. Calculate the wavelength of the X-ray radiations. (Ans. 0.86 Å)

9. The primitive translation vectors of the hexagonal space lattice are

$$\vec{a} = 2\hat{i} + \hat{j}$$

$$\vec{b} = 2\hat{j}$$

$$\vec{c} = \hat{k}$$

Find (i) the volume of the primitive cell of direct lattice.

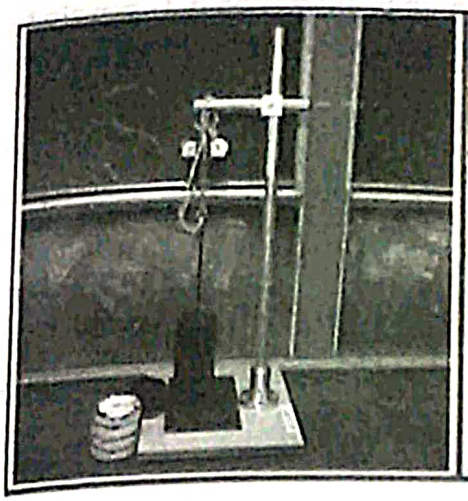
(ii) primitive translation of the reciprocal lattice. (Ans. Volume =

$$\vec{A} = \pi\hat{i}\ \ \vec{B} = \frac{1}{2}\pi(-\hat{i} + 2\hat{j})\ \ \vec{C} = 2\pi k$$

10. X-rays of wavelength 1.5 Å make a glancing angle of 16° in the first order whe diffracted from NaCl crystal. Find the lattice constant of NaCl. (Ans. 2.72 Å)

11. If X-rays of wavelength 0.5 Å are diffracted at an angle of 5° in the first order, wh is the spacing between the adjacent planes of the crystal. At what angle will secon maximum occur ? (Ans. 10.0

□□□



Chapter 2

ELEMENTARY LATTICE DYNAMICS

2.1 INTRODUCTION

Lattice dynamics is an important aspect of the study of solid state physics. While studying the structure of the crystals we had assumed the atoms in the crystal to be at rest whereas in actual practice atoms vibrate about the mean position. These vibrations of atoms cause thermal properties such as heat capacities, thermal conductivity, thermal expansion etc.

In this chapter we will study the properties of elastic vibrational motion of the crystal lattice. We will first study the normal modes of vibration. Then the results obtained for one dimensional case will be extended to two and three dimensional lattices. Only longitudinal mode in which atoms will be vibrating parallel to the external applied force will be considered. We shall also study the concepts of phonons and specific heat theories given by Einstein and Debye.

2.2 LATTICE VIBRATIONS

Every atom has a tendency to vibrate about their mean position at temperature above zero Kelvin. The mean position is referred as the Bravais lattice site. These vibrations occur due to interatomic interactions. As the atoms in the solid are present at lattice sites, so these vibrations are called Lattice vibrations.

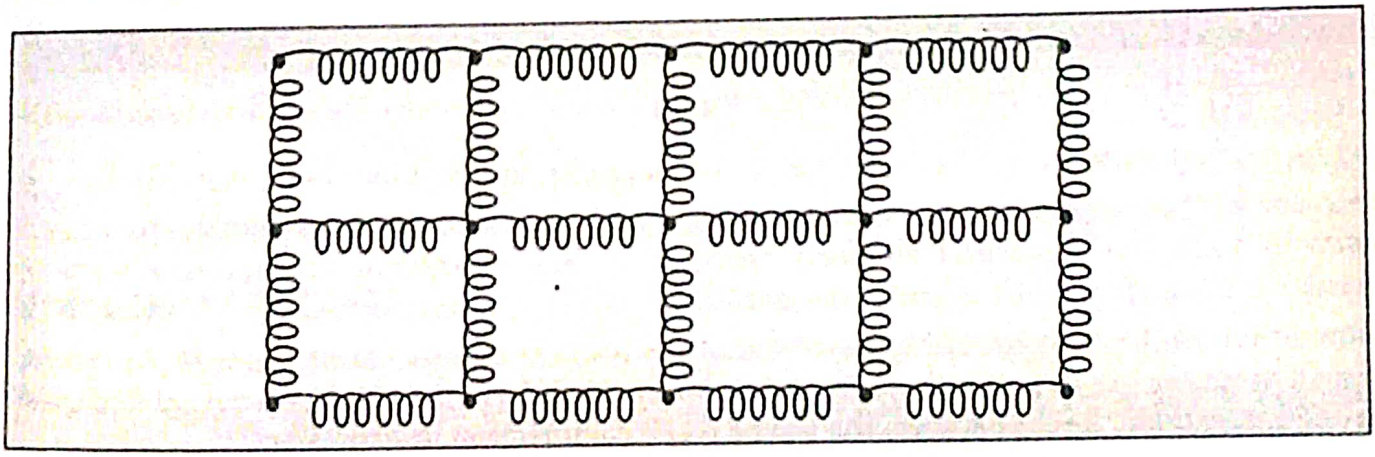


Fig. 2.1

The lattice vibrations are the result of absorption of heat energy. A lattice is an array of atoms connected with each other by elastic springs or strings as shown in Fig. 2.1. Here all

the atom present at lattice site are coupled and the motion of one single atom is shared by the neighbouring atoms. Thus the crystal vibrates on a whole. The dynamic external forces which are responsible for the vibrations obey Hooke's law. It is assumed that the amplitudes of the vibrations are small as compared to the interatomic spacing. Harmonic approximation is valid for lattice vibrations. Thus every atom present at lattice site is considered to be as harmonic oscillator.

According to quantum theory, the energy E of an elastic mode of vibration of angular frequency when the mode is excited to a quantum number n is given as

$$E = \left(n+\frac{1}{2}\right)\hbar\omega$$

$$= n\hbar\omega+\frac{1}{2}\hbar\omega$$

Here $\frac{1}{2}\hbar\omega$ is the zero point energy and $n\hbar\omega$ represents the quanta of energy which is called phonon energy.

To understand the lattice vibration, let us revise interatomic forces near the neighbourhood of equilibrium separation about which the atoms vibrate. The interatomic forces may be attractive or repulsive depending upon the separation between the two atoms (Fig. 2.2).

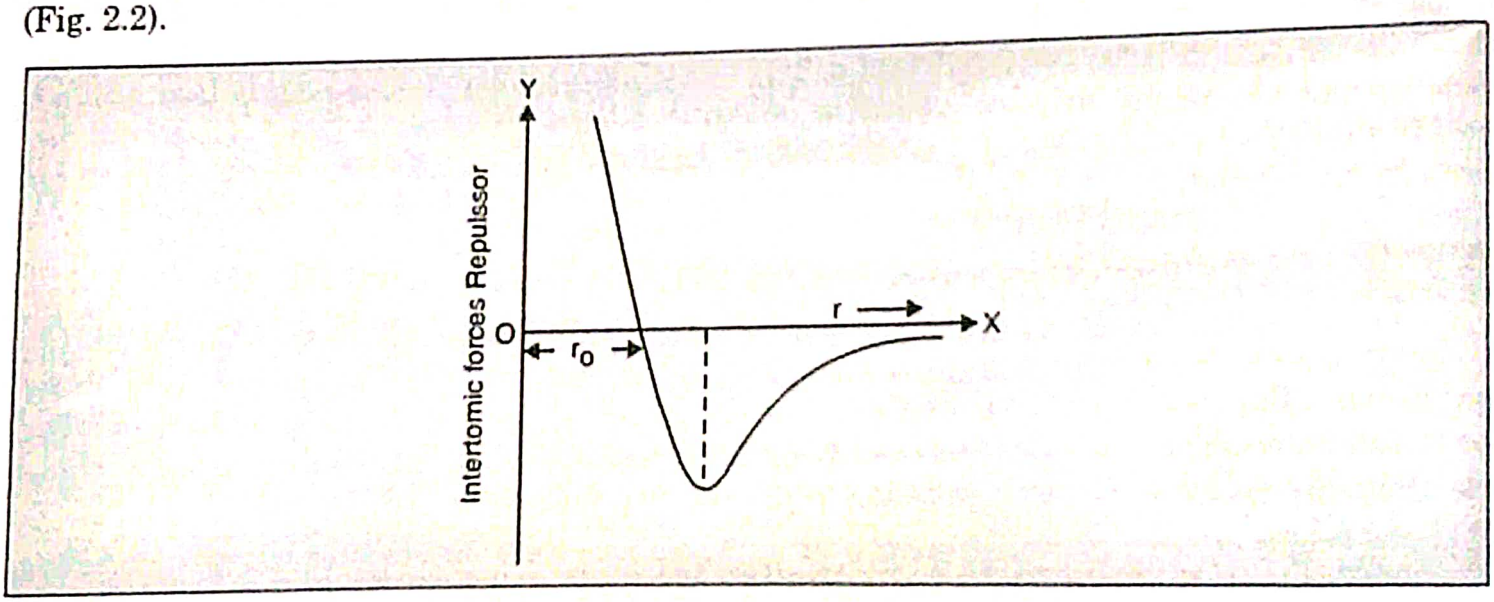


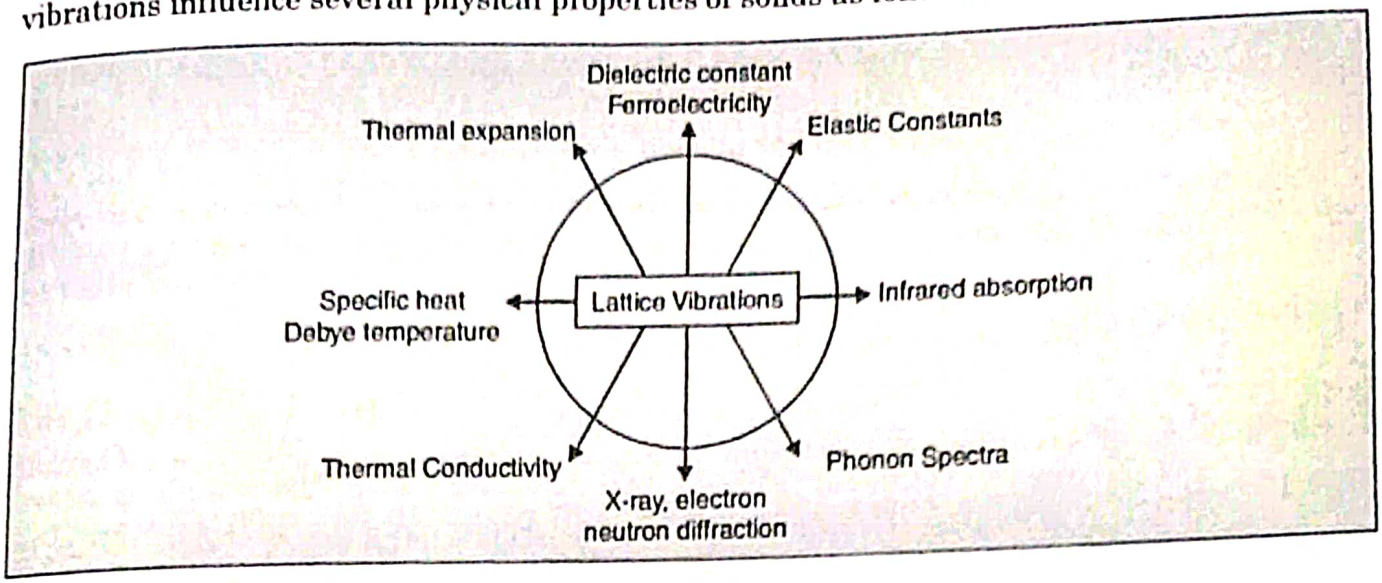
Fig. 2.2

At normal distance r_0, the two atoms are placed at equilibrium space. Any increase or decrease in their separation, needs some energy. An increase in the interatomic separation r leads to attractive force and similarly decrease in the interatomic separation r leads to repulsive force. For NaCl crystal, the normal distance r_0 is approximately 1Å which is of same order as the distance from the centre of the atom to its outermost electron. As the Na and Cl atoms exists in a regular array, when we try to deform the solid by external force, the strong interatomic forces between the atoms resist compression or extension.

A regular lattice with harmonic forces between atoms and normal modes of vibration are called lattice waves. Lattice waves have frequencies from low value to high values of the order 10 Hz. The wavelengths corresponding to high frequencies are comparable to the

interatomic spacing. Due to short wavelengths the motion of the neighbouring atoms is uncorrelated, with each atom vibrating about mean position in three dimensions with average vibrational energy. The electrical resistance in the conducting solids arise due to the interaction of lattice vibrations with free electrons.

The theories of lattice vibrations are associated with the specific heat of solids. These vibrations influence several physical properties of solids as follows :



2.3 PHONONS

The energy in a lattice vibration or an elastic wave is quantised. This is similar to the quantisation of electromagnetic energy. Whereas the quantum of electromagnetic energy is called photon, the quantum of the lattice energy is known as **phonon.** A photon travels with the velocity of light whereas the phonon with the velocity of sound in a solid. Remember, photons do not require any material medium for their propagation whereas phonons do need a material medium to travel. Thus, phonons can never travel through a vacuum.

Mathematically, the energy of lattice vibrations or phonon is given by

$$E = \hbar\omega$$

Where $\hbar = \frac{h}{2\pi}$, h being Planck's constant and ω is the angular frequency of vibration.

When space lattice is excited in n^{th} state, then n phonons each of energy $\hbar\omega$ are present. One phonon is released when the lattice transists from n^{th} mode to $(n + 1)^{th}$ mode. Similarly during the transistion from n^{th} mode to (n–1)th mode, a phonon is said to be destroyed. In this way, phonons are created and destroyed during the transition of lattice from one mode of vibration to another.

Properties of a Phonon :

(i) Phonon is produced as a result of the quantisation of lattice vibration.

(ii) Phonon possess both wave as well as particle nature. In other words, we conclude that the wave particle duality also applies to phonon.

(iii) Phonons like photons have zero spin. Therefore phonons follows Bose-Einstein statistics and are indistinguishable particles.

(iv) The momentum of a phonon is called crystal momentum. It is represented as $\hbar k$ where k is a wave vector. In physical sense, a phonon on a lattice really has no momentum but when its particle nature is taken into account during the interaction with photon, electron and neutron, it behaves as if it possesses momentum.

(v) The energy of a phonon is given by

$$E = \hbar\omega$$

$$= hfk$$

where f is the frequency and k is phonon wave vector.

(vi) Due to Bose-Einstein's distribution law, the increase in temperature of crystal enhances the number of phonons and decrease in temperature destroys the phonons.

(vii) The pictorial representation of a phonon is shown in Fig. 2.3 as

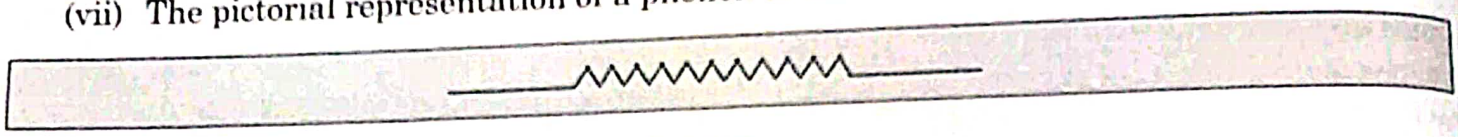


Fig 2.3

(viii) The phonons do not conserve in number as they can be created or destroyed.

(ix) The vibration spectrum of the phonon wave occupies a wide range of frequencies from 10^4 to 10^{12} Hz.

(x) The low frequency part of the spectrum corresponds to acoustic region and comprises sound waves in a crystal lattice.

(xi) The high frequency part of the spectrum lies in the infrared region and is due to thermal vibrations in a crystal similar to the thermally excited photons in black body radiations.

(xii) Phonon travel with velocity of sound in the solid.

Point to Remember

The concept of phonons was introduced in 1932 by Soviet physicist Igor Tamm (1895–1971), who was awarded Nobel prize in physics in 1958.

The name phonon comes from Greek word phone which means sound or voice. This is because long wavelength phonons give rise to sound.

(xiii) The number of phonons in a crystal is temperature dependent.

(a) At finite temperatures, the crystals are full of phonons.

(b) At low temperatures, acoustic modes are more populated than the optical modes.

(c) At high temperatures, the atomic vibrations amplitude increases.

In the case of Bragg's diffraction i.e. in an elastic scattering of X-ray photon by a crystal, we have

$$\vec{K}' = \vec{K} + \vec{G}$$

where $\vec{K}$ and $\vec{K}'$ are the incident and scattered wave vectors. G is the reciprocal lattice vector of the crystal. Multiply both sides by $\hbar$, we have

$$\hbar\vec{K}' = \hbar\vec{K} + \hbar\vec{G}$$

or $$\hbar(\vec{K}' - \vec{K}) = \hbar\vec{G}$$

Here, the entire crystal recoils with momentum $\hbar\vec{G}$. In the case of elastic scattering the frequency of the scattered photon is same as that of the incident photon.

This type of process in which the frequency of the incident photon is the same as that of the scattered photon is known as **Normal process or N-process.** In this process no phonon is created or destroyed.

In an inelastic scattering of a photon by a crystal, the frequency of the incident photon changes and a new photon is emitted alongwith an emitted or absorbed phonon. Let $\vec{k}$ be the wave vector of a phonon emitted or created during the scattering, then due to the conservation of wave vector, we have

$$\vec{K}' \text{ (Scattered)} + \vec{k} = \vec{K} \text{ (incident)} + \vec{G}$$

or $$h\vec{K} + h\vec{k} = h\vec{K} \text{ (incident)} + h\vec{G}$$

If a phonon of wavevector $\vec{k}$ is absorbed during the scattering, then according to the wave vector conservation law,

$$\vec{K}' \text{ (Scattered)} = \vec{K} \text{ (incident)} + \vec{k} + \vec{G}$$

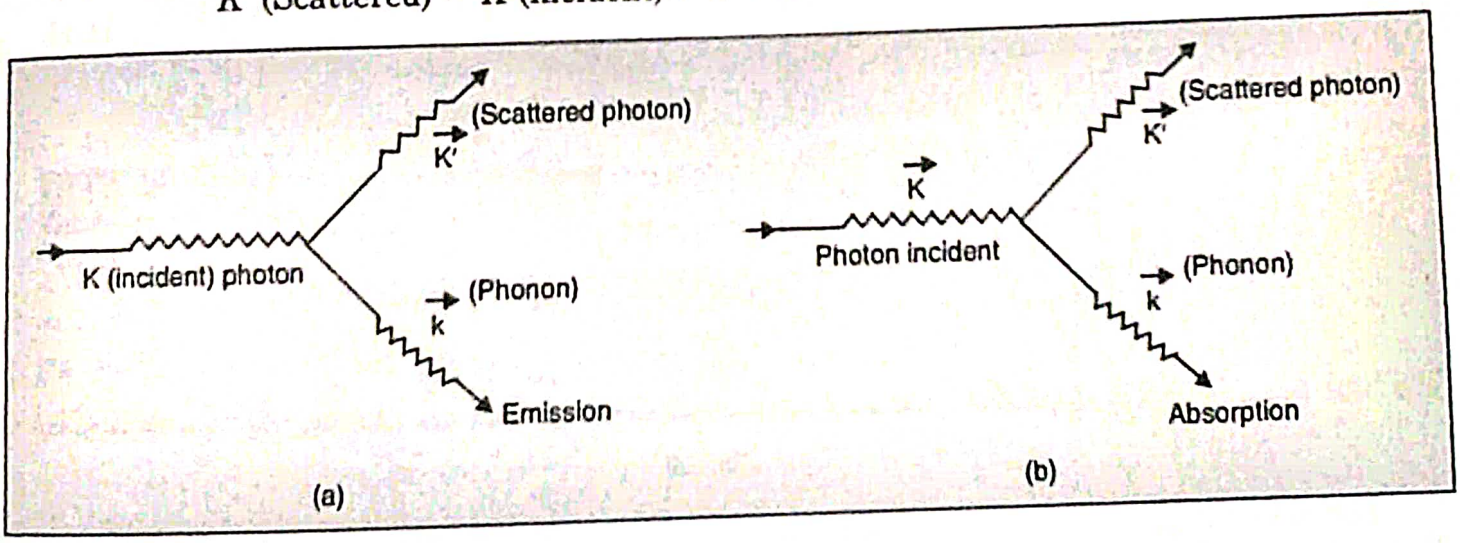


Fig. 2.4

The emission and absorption of phonon in inelastic scattering is shown in Fig. 2.4 (a) and (b).

This type of a process in which the frequency of the photon changes is known as **Umklapp process or U-process.** Umklapp is a German word which means flipping over. Apart from Bragg's reflection, a phonon is created or absorbed in this process. Tne momentum is transferred to the crystal as a whole.

Inelastic scattering of photons by phonons. In the case of elastic scattering of X-ray photons, only a change in the direction of wave vector $\overline{K}$ of the incident photon takes place but the magnitude of the wave vector is not changed.

When inelastic scattering of a photon by a crystal takes place, the frequency of the incident photon also changes and a phonon is either emitted or absorbed in accordance with the principle of conservation of energy, we have

Energy of the incident photon = Energy of the scattered photon + Energy of emitted phonon

Let a photon of frequency f propagate phonon in a crystal. The wave vector of the photon is given by

$$\vec{k} = \frac{2\pi}{\lambda}$$

$$= \frac{2\pi\mu\omega}{C}, \text{ where } \mu \text{ is the refractive index.}$$

$$\vec{k} = \frac{\omega\mu}{C}$$

Also, in accordance with the principle of conservation of momentum, we have

Momentum of the incident photon = Momentum of scattered photon + Momentum of emitted phonon.

Let the photon interact with a phonon beam in the crystal and gets scattered as shown in Fig. 2.5.

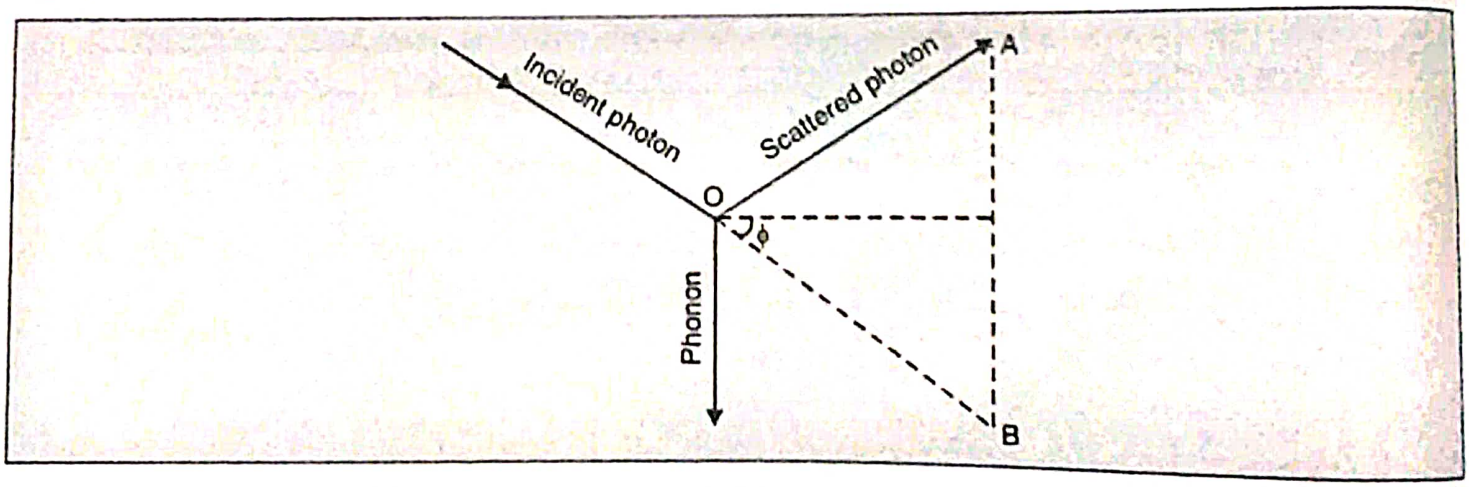


Fig. 2.5

The scattering of photon takes place due to change in the refractive index of the crystal. The refractive index changes due to the change in concentration of atoms brought about by the elastic strain field of the sound waves. In the inelastic scattering of the photon, a phonon is either created or absorbed. Let the wave vector of the photon change from, $\overline{K}$ to $\overline{K}'$ and the frequency from ω to ω' due to inelastic scattering. The phonon which is created during the scattering has a wave vector $\bar{k}$ and frequency Ω. Then, as per the law of conservation of energy.

$$\hbar\omega = \hbar\omega' + \hbar\Omega$$

and as per the law of conservation of momentum, we have

$$\hbar\vec{K} = \hbar\vec{K}' + \hbar\vec{k}, \text{ where } \hbar = \frac{h}{2\pi}$$

Let $\vec{v}$ be the velocity of sound, then

$$\vec{v} = \frac{\Omega}{2\pi} \times \frac{2\pi}{k}$$

$$= \frac{\Omega}{k}$$

or $$\Omega = \vec{v}\,\vec{k}$$

where Ω is the angular frequency of phonon of wave vector of magnitude k.

The phonon which is emitted carries a very small part of the incident energy of the photon. We know that the velocity of sound $\vec{v}$ is very less in comparison to the velocity of light c, so, we have,

$$v\,\vec{k} << c\,\vec{k}$$

Also $$\omega = c\,\vec{k} \text{ and } \Omega = v\,\vec{k}$$

Hence the angular frequency ω is very very large in comparison to the angular frequency Ω of the phonon.

Taking $\omega' = \omega$ and $\vec{K}' = \vec{K}$, we have form Fig. 2.5

OA = OB such that ΔOAB is an isosceles triangle.

Hence, $$AB = |\,k\,| = 2K \sin\phi$$

where $$\angle AOB = 2\phi \text{ and } OC \perp AB$$

Also, we know $$\vec{K} = \frac{\omega\mu}{c} \sin\phi$$

hence, $$k = \frac{\omega\mu}{c}$$

and $$\Omega = v\,\vec{k}$$

$$= \frac{2v\omega\mu}{c} \sin\phi$$

Close agreement of the theoretical and experimental results for Ω indicates a very strong evidence of the existence of phonons and their behaviour.

2.4 LINEAR MONOATOMIC VIBRATIONS

Let us assume that

(i) Atoms are arranged linearly in a straight line.

(ii) The interatomic spacing (a) is constant.

(iii) The mass (m) of each atom in the crystal is same.

(iv) The atom is supposed to be a rigid sphere in the crystal.

(v) The crystal is under the influence of short range forces where the interactions between atoms are confined to only the nearest neighbour.

(vi) Each atom in one dimensional monoatomic lattice is connected with a spring having spring constant α and the spring is massless.

(vii) The force on the atom is directly proportional to the extension or contraction of its nearest neighbouring distance.

(viii) All the atoms in linear array obey Hooke's law.

(ix) For simplicity we consider only the longitudinal mode of vibrations.

(x) A linear chain of identical atoms extend along the X-axis as shown in Fig. 2.6.

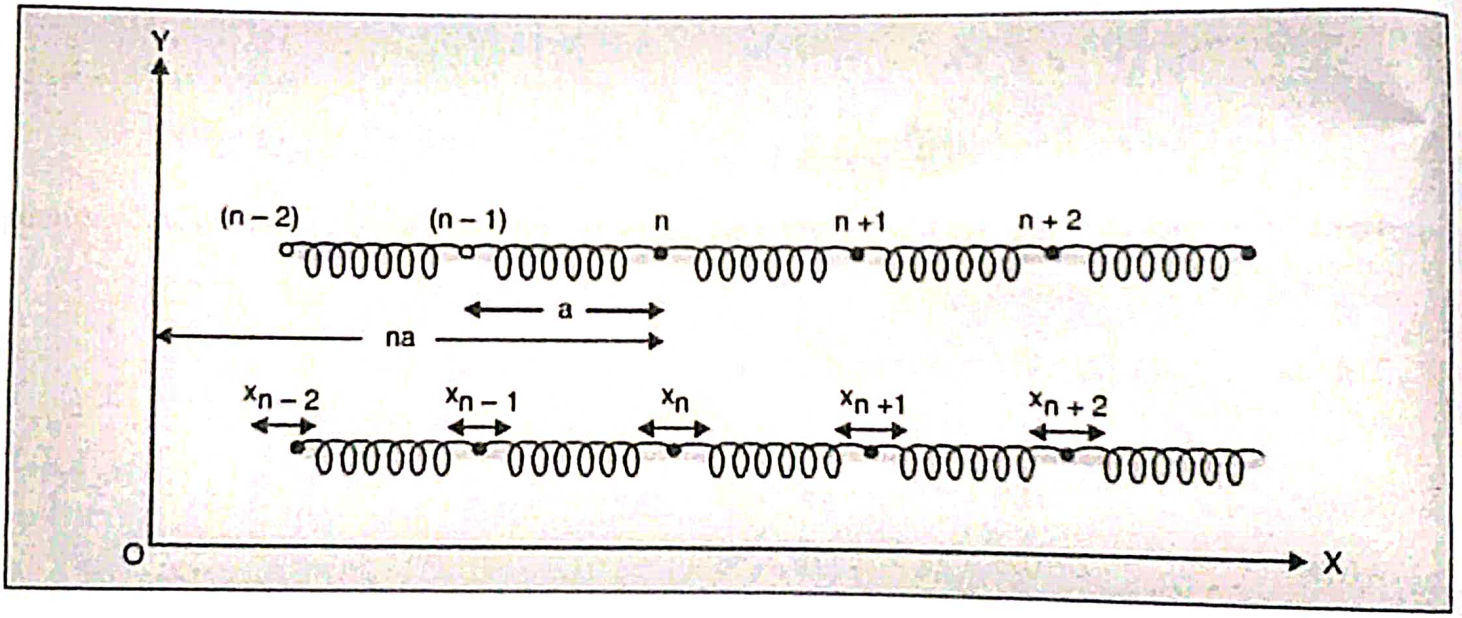


Fig. 2.6

At mean position, the distance of n^{th} atom from the origin is (na). When the crystal lattice starts vibrating, the atoms gets displaced by a small magnitude. Let x_{n-2}, x_{n-1}, x_n, x_{n+1}, x_{n+2} etc. be the displacements of $(x-2)^{th}$, $(n-1)^{th}$, n^{th}, $(n+1)^{th}$, $(n+2)^{th}$ etc. atoms respectively from their respective mean positions. The spring joining n^{th} and $(n+1)^{th}$ atom extends by $(x_{n+1} - x_n)$ and exerts force $\alpha(x_{n+1} - x_n)$ on n^{th} atom and exerts the force $(x_n - x_{n-1})$ on n^{th} atom in opposite direction. Hence the net force on the n^{th} atom is

$$\vec{F} = \alpha (x_{n+1} - x_n) - \alpha (x_n - x_{n-1})$$

$$= \alpha (x_{n+1} + x_{n-1} - 2x_n) \quad \ldots(i)$$

Applying Newton's second law of motion to n^{th} atom, we get

$$\frac{m\,d^2x_n}{dt^2} = \alpha\,(x_{n+1} + x_n - 2x_n) \qquad \ldots(ii)$$

The solution of above differential equation is expressed as

$$x_n = A\,e^{i\,(kna - \omega t)} \qquad \ldots(iii)$$

where A is the amplitude of the resultant wave and ω is the angular frequency of the travelling wave in which all the atoms oscillate k is the propagation constant which is equal to $2\pi/\lambda$ and λ is the wavelength of the resultant wave. Remember although the amplitude A remain same but the different atoms in the crystal vibrate in different phase which increases quickly from one atom to next by amount (ka).

Differentiating equation (iii) twice with respect to time, we obtain acceleration as

$$\frac{d^2x_n}{dt^2} = i^2\omega^2 A\,e^{i\,(kna - \omega t)}$$

$$= -A\,\omega^2 e^{i\,(kna - \omega t)}$$

The displacement of $(n-1)^{th}$ atom and $(n+1)^{th}$ atom can be expressed as

$$x_{n-1} = A\,e^{i\,[k(n-1)\,a - \omega t]}$$

and $$x_{n+1} = A\,e^{i\,[k(n+1)\,a - \omega t]}$$

Substituting, the values in equation (ii) we have

$$-m\,A\,\omega^2\,e^{[i\,(kna - \omega t)]} = \alpha\,A\,e^{i\,[k(n-1)\,a - \omega t]} + \alpha\,A\,e^{[ik(n-1)\,a - \omega t]}$$

$$- 2\,\alpha\,A\,e^{[i\,(kna - \omega t)]}$$

$$-m\omega^2 = \alpha[e^{ika} + e^{-ika} - 2]$$

$$= \alpha\left[2\,i\,\sin\left(\frac{ka}{2}\right)\right]^2$$

or $$-m\omega^2 = -\alpha 4\left[\sin\left(\frac{ka}{2}\right)\right]^2$$

$$\omega^2 = \frac{4\alpha}{m}\left[\sin\left(\frac{ka}{2}\right)\right]^2$$

or $$\omega = 2\sqrt{\frac{\alpha}{m}}\,\sin\left(\frac{ka}{2}\right)$$

$$= \omega_0\,\sin\left(\frac{ka}{2}\right) \qquad \ldots(iv)$$

This is called the **dispersion relation** because it relates ω to the propagation constant k. For simplicity, we consider only the positive root of above equation so as to have real frequencies.

Here, ω_0 the maximum angular frequency of the vibrating atoms and is given by

$$\omega_0 = 2\sqrt{\frac{\alpha}{m}}$$

Knowing the mass of the atoms from standard values, we can obtain the expression for the frequency f, called the **Einstein's frequency**

$$f = \frac{1}{2\pi}\sqrt{\frac{\alpha}{m}}$$

As an example, consider atom of *Cu, Fe, Ge* etc. whose atomic masses are approximately 10^{-25} *kg*. The frequency of these atoms comes out to be close to 3×10^{12} *Hz*. If the value of $\alpha \approx 25$ Nm^{-1} then the frequency f is nearer to 10^{13} *Hz* approx.

If we plot a graph between propagation constant or a wave vector k along X-axis and corresponding values of angular frequency ω along Y-axis for a longitudinal wave of a linear one dimension lattice, then the dispersion curve will look like as in Fig. 2.7.

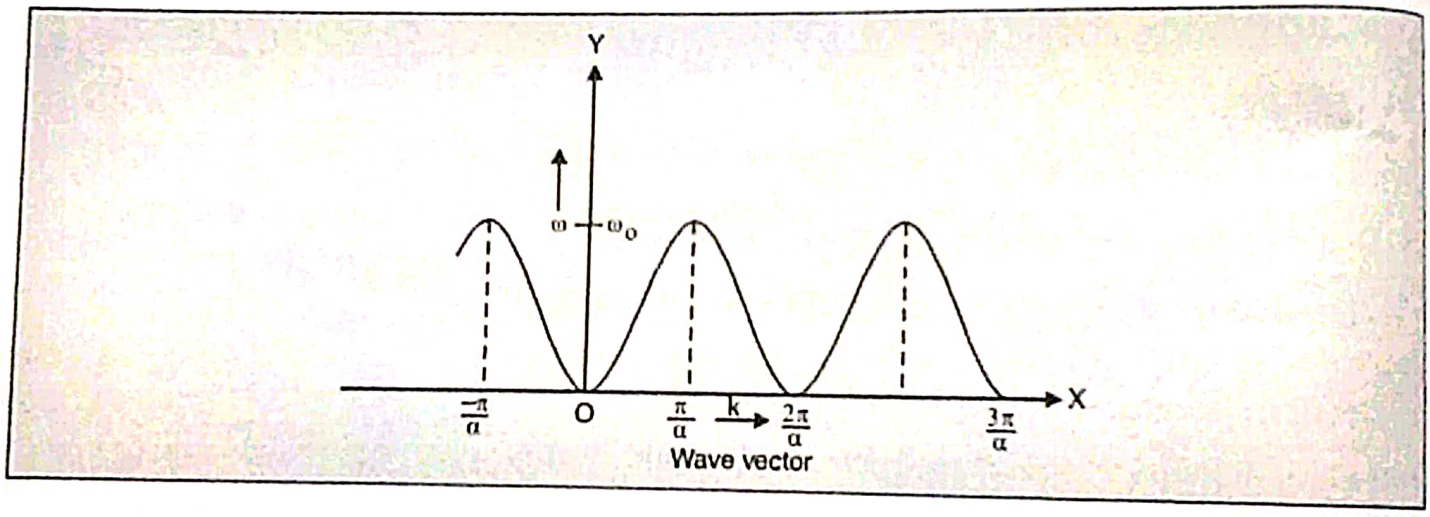


Fig. 2.7

A correlated motion of the atoms which has a characteristic wave vector $\vec{k}$ and angular frequency ω is known as **normal mode** of a lattice. Once this motion gets started, it will go on continuously, provided the dissipative forces such as friction are negligible. The powerful bonds transmit the vibrations of one atom to other atom so as to have a collective motion in the form of an elastic wave. This collective motion of atoms is referred as the normal mode of a lattice. The number of normal modes coincides with the number of degrees of freedom. The degrees of freedom is equal to $3N$ where N is the number of atoms constituting the crystal.

The one-dimensional model of a solid shown in Fig. 2.6 can be redrawn as in Fig. 2.8(*a*). The chain shown in Fig. 2.8(*a*) may be supposed to be a string. If the ends of chain are fixed, then the fundamental mode corresponding to the lowest frequency ω_{min} is shown by the stationary wave with a node at each end in the curve 1 in Fig. 2.8(*b*). The second mode is shown by the stationary wave with an additional mode in the centre of chain as in curve 2 of Fig. 2.8(*b*). The third harmonic or the third mode is shown by the stationary wave with two

additional nodes that divide the chain in three equal parts as in curve 3 of Fig. 2.8(*b*). The length of the shortest wave in such a chain is equal to double the distance of lattice length *a*. *i.e.*

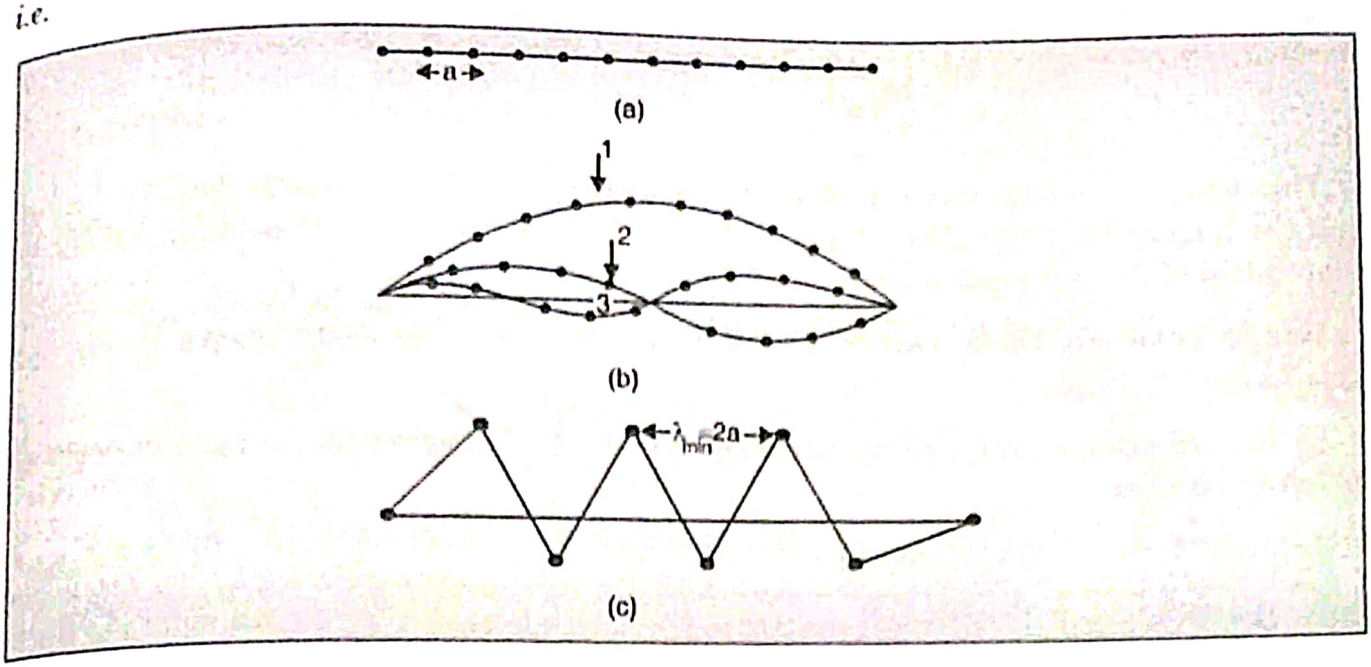


Fig. 2.8

$$\lambda_{min} = 2a$$

The corresponding maximum frequency ω_0 is

$$\omega_0 = \frac{2\pi v}{\lambda_{min}} = \frac{\pi v}{a}$$

where v is the velocity of the propagation of longitudinal wave along the chain.

As an illustration, if $a = 3.6 \times 10^{-10}$ *m*, and $\vec{v} = 3550\ ms^{-1}$ in the case of copper material then the maximum value of angular frequency comes out to be 3096×10^{10} rad s^{-1}, which is comparable to the frequency of atomic vibration in a solid.

The Importance of Normal Mode : In classical physics, we study that if one mode is set into vibrations, then it continues to vibrate indefinitely while the others remain unexcited. In quantum mechanics, the normal mode decomposition is possible only because the equations of motion for the atomic displacements are linear in all of the displacement. Higher order terms are required for understanding many important processes. The apparent breakdown of the harmonic approximation leads to measurable effects such as phonon-phonon interactions.

The energy of the j^{th} normal mode E_j is quantised and is given by

$$E_j = \left(n_j + \frac{1}{2}\right) \hbar \omega_j$$

where $n_j = 0, 1, 2, \ldots\ldots$, while the net energy of the system is the sum of the individual energies as per the principle of superposition.

$$E_{net} = \sum_j E_j$$

when $n_j = 0$, the energy corresponds to zero point energy,

$$E_{j,0} = \frac{1}{2}\hbar\omega_j$$

This zero point energy does not affect the physical results. As this energy does not depend upon the temperature, the calculations of specific heat of substances at constant volume is independent of the zero point energy.

Graph between wave vector k and frequency ω : The graph shown in Fig. 2.1 explains the following :

(*i*) The reflection symmetry exists between k and $-k$. The waves travelling to the right to the left are similar

i.e. $$\omega(k) = \omega(-k)$$

(*ii*) The periodic symmetry exists as the results repeat with a period of $\frac{2\pi}{a}$.

i.e. $$\omega\left(k \pm \frac{2\pi}{a}\right) = \omega(k)$$

(*iii*) There exists a maximum or cutoff frequency ω_0, above which the chain of atoms cannot sustain a travelling wave.

ω_0 occurs at $k = \left(\frac{\pi}{a}\right) + \left(p\frac{2\pi}{a}\right)$ where p is any integer and its value is equal to,

$$\omega_0 = 2\sqrt{\frac{\alpha}{m}}$$

One dimensional chain of identical particles allows the propagation of frequencies lying in the range from zero to ω_0 and the upper range is infrared region.

(*iv*) $\omega - k$ graph is called dispersion curve graph because the linear relation between ω and k does not hold, *i.e.*, the crystalline substance is dispersive in nature.

(*v*) For small values of ka, we have

$$\omega \cong \left(\frac{\alpha}{m}\right)^{1/2} ak$$

or $$\left(\frac{\omega}{k}\right) = \left(\frac{\alpha}{m}\right)^{1/2} a$$

The term on the left hand side $\left(\frac{\omega}{k}\right)$ is the **phase velocity** v_p, so we have

$$\vec{v}_p = \left(\frac{\alpha}{m}\right)^{1/2} a$$

(*vi*) For monoatomic linear chain between $k = 0$ and $\frac{\pi}{a}$, the group velocity v_g is given by the relation

$$v_g = \frac{d\omega}{dk}$$

Putting $\omega = 2\sqrt{\frac{\alpha}{m}} \sin\left(\frac{k}{2}\right)$ and differentinting v_g with respect to k, we get

$$v_g = \left(\frac{\alpha}{m}\right)^{1/2} a \cos\left(\frac{ka}{2}\right)$$

The graph between k and v_g is shown in Fig. 2.9.

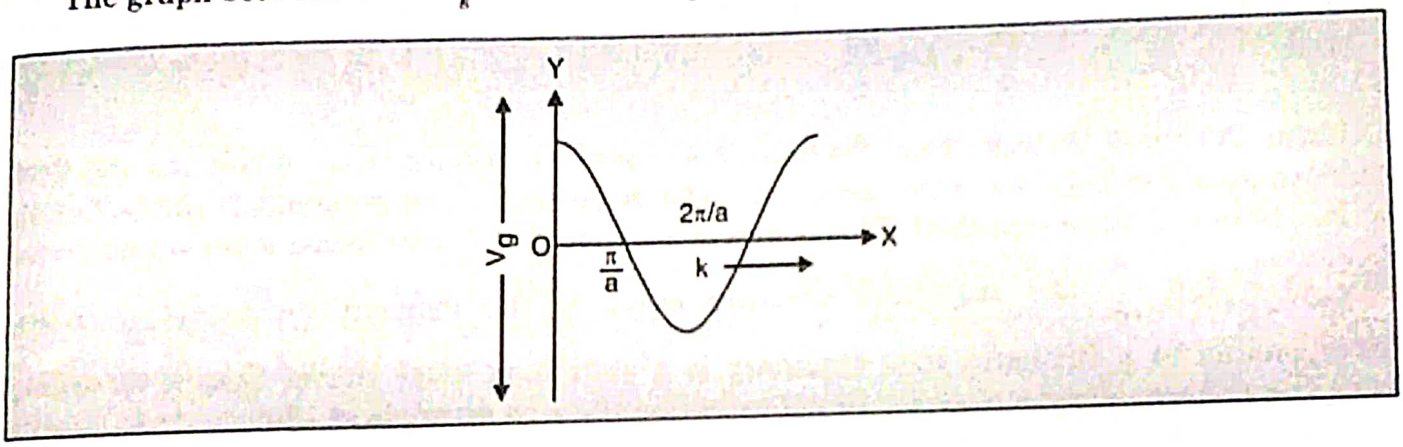


Fig. 2.9

Physical significance of group velocity is that it a velocity with which the energy in the wave group is transmitted. For a monochromatic wave, group velocity and phase velocity are same. Thus for small values of k, $v_g \simeq v_p$ and for $k = \frac{\pi}{a}$, v_g becomes equal to zero.

In general, $v_g = 0$, whenever $k = \frac{\pi}{a} + p$ where p is any integer. This k-periodic dispersion curve is the consequence of the translational symmetry of the crystal.

(*vii*) These vibrational modes discussed in sr. no (*vi*) are called acoustic modes and the study of ω *v/s* k shown in Fig. 2.7 is known as acoustic study because at small values of k, there is a constant non-zero group velocity. The name acoustic branch is assigned because it gives rise to long wavelength vibrations.

(viii) Brillouin Zones : The frequency corresponding to the modes k and k_p are identical when $k = k_p = \frac{2\pi p}{a}$ where $p = 1, 2, 3, \ldots\ldots$. The wave vector k and the state of vibration of lattice has a unique relationship when the lattice is confined to a range of values $\frac{2\pi}{a}$, such that

$$\frac{-\pi}{a} \leq k \leq \frac{\pi}{a} \qquad \ldots(v)$$

The positive values of k represent the wave propagating in one direction whereas the negative values of k represent waves going in opposite direction. The region of k values in accordance with the conditions shown in eqn. (v) is called the **first Brillouin zero.**

The second Brillouin zone consists of two regions

$$\frac{-2\pi}{a} \leq k \leq \frac{-\pi}{a}$$

and

$$\frac{\pi}{a} \leq k \leq \frac{2\pi}{a}$$

The two regions

$$\frac{-3\pi}{a} \leq ki \leq \frac{-2\pi}{a}$$

and

$$\frac{2\pi}{a} \leq k \leq \frac{3\pi}{a},$$

forms the third Brilluin zone. Because of the periodic nature of ω - k relation the first Brillouin zone contains the entire spectrum. The dispersion curve gradually becomes flat as the Brillouin zone is approached. This is due to a component of a reflected wave which grows until at $k = \pm \frac{\pi}{a}$ the amplitude becomes equal to the incident component. A wave corresponding to a Brillouin zone boundary is a stationary wave rather than a travelling wave. It has a wavelength close for Bragg reflection through an angle of 180°.

2.5 VIBRATIONS OF DIATOMIC CHAINS

Let us take case of one dimensional diatomic lattice which has two atoms per primitive cell as in case of sodium chloride or the diamond structure. Let m_1 and m_2 be the mass of these two atoms and suppose that $m_1 < m_2$. The distance between two nearest neighbours be a. Suppose the atoms are arranged along X-axes and are placed at lattice sites $2n - 3$, $2n - 2$, $2n - 1$, $2n$, ... etc. The atoms having smaller mass are placed at even numbered sites and atoms with larger mass are placed at odd numbered sites as shown in Fig. 2.10. The assumptions are supposed to be same as that for monoatomic lattice except that let x_{2n} represent displacement of atom at $2n^{th}$ site.

In strained state shown in Fig. 2.10(b) the equation of motion of the two atoms can be written as

$$m_1 \frac{d^2x_{2n}}{dt^2} = \alpha\,(x_{2n+1} + x_{2n-1} - 2x_{2n}) \qquad \ldots(i)$$

and

$$m_2 \frac{d^2x_{2n+1}}{dt^2} = \alpha\,(x_{2n+2} + x_{2n} - 2x_{2n+1}) \qquad \ldots(ii)$$

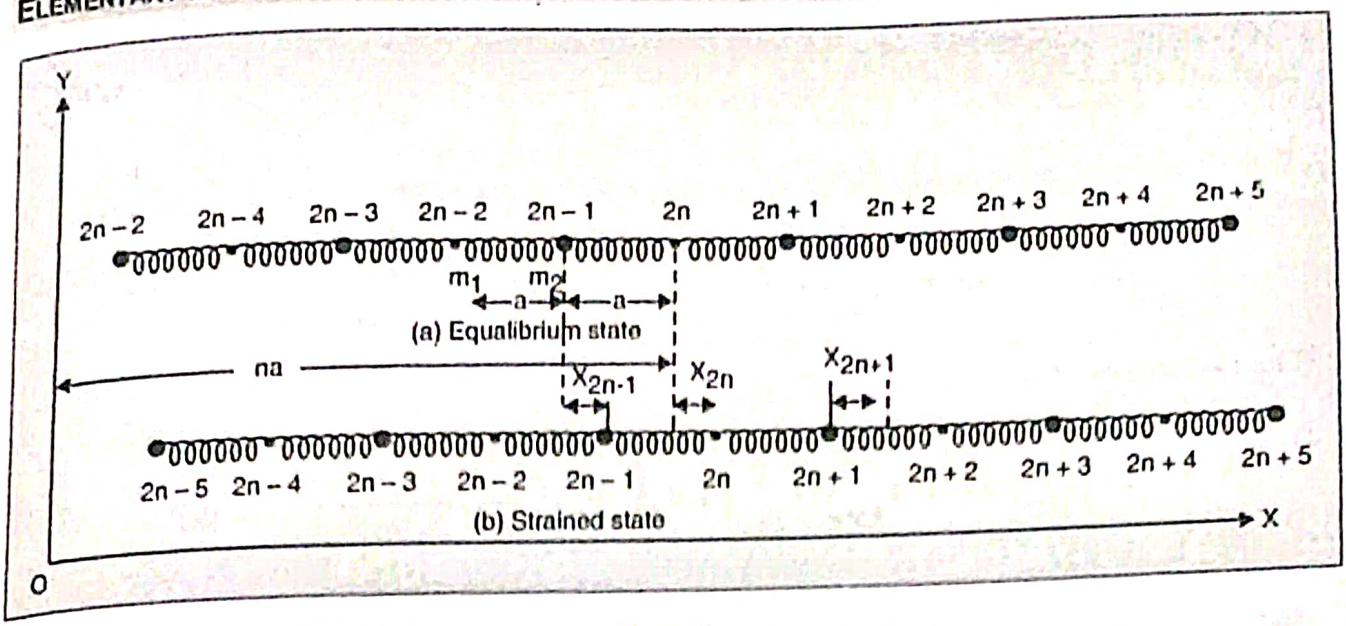


Fig. 2.10

where α is the interatomic force constant. The solutions of equation (*i*) and equation (*ii*) can be written in the form as

$$x_{2n} = A\, e^{i\,(2kna - \omega t)} \qquad \ldots(iii)$$

and

$$x_{2n+1} = B\, e^{i\,[(2n+1)\,ka - \omega t]} \qquad \ldots(iv)$$

In diatomic lattice, the two masses are not identical, so their amplitudes of vibrations are taken to be different. Since both the masses are vibrating in identical manner, the frequency of both the atoms is taken to be same.

Differentiating eqns. (*iii*) and (*iv*) twice and substituting the respective values in eqns. (*i*) and (*ii*) we have,

$$-m_1\omega^2 A = \alpha\,[e^{ika} + e^{-ika}]\,B - 2\,\alpha\,A \qquad \ldots(v)$$

$$-m_2\omega^2 B = \alpha\,[e^{ika} + e^{-ika}]\,A - 2\,\alpha\,B \qquad \ldots(vi)$$

We know that

$$e^{ika} + e^{-ika} = 2\cos(ka)$$

So that eqns. (*v*) and (*vi*) an be rewritten as

$$(2\alpha - m_1\omega^2)\,A - 2\alpha\,(\cos ka)\,B = 0$$

$$-2\alpha\,(\cos ka)\,A + (2\alpha - m_2\omega^2)\,B = 0$$

$$\text{or} \begin{bmatrix} (2\alpha - m_1\omega^2) & -2\alpha\,(\cos ka) \\ -2\alpha\,(\cos ka) & (2\alpha - m_2\omega^2) \end{bmatrix} \cdot \begin{bmatrix} A \\ B \end{bmatrix} = 0$$

The expansion of above determinant gives

$$(2\alpha - m_1\omega^2)\,(2\alpha - m_2\omega^2) - 4\alpha^2\cos^2 ka = 0$$

$$\text{or}\ \omega^2 - \frac{2\alpha(m_1 + m_2)}{m_1 m_2}\omega^2 + \frac{4\alpha^2 \sin^2 ka}{m_1 m_2} = 0$$

The above equation is quadratic in ω^2, solving it for ω^2, we have

$$\omega^2 = \alpha\left(\frac{1}{m_1} + \frac{1}{m_2}\right) \pm \alpha\sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2}\right)^2 - \frac{4\sin^2 ka}{m_1 m_2}}$$

The two values of ω^2 are

$$\omega_+^2 = \alpha\left(\frac{1}{m_1} + \frac{1}{m_2}\right) + \alpha\sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2}\right)^2 - \frac{4\sin^2 ka}{m_1 m_2}}$$

and

$$\omega_-^2 = \alpha\left(\frac{1}{m_1} + \frac{1}{m_2}\right) - \alpha\sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2}\right)^2 - \frac{4\sin^2 ka}{m_1 m_2}}$$

Above two equations are called dispersion relations for one dimensional diatomic lattice.

2.6 ACOUSTICAL AND OPTICAL PHONONS

The graph between ω and k gives us two branches of the dispersion relation curve. One curve corresponding to ω_- is called acoustical branch and the other corresponding to ω_+ is called optical branch as shown in Fig. 2.11.

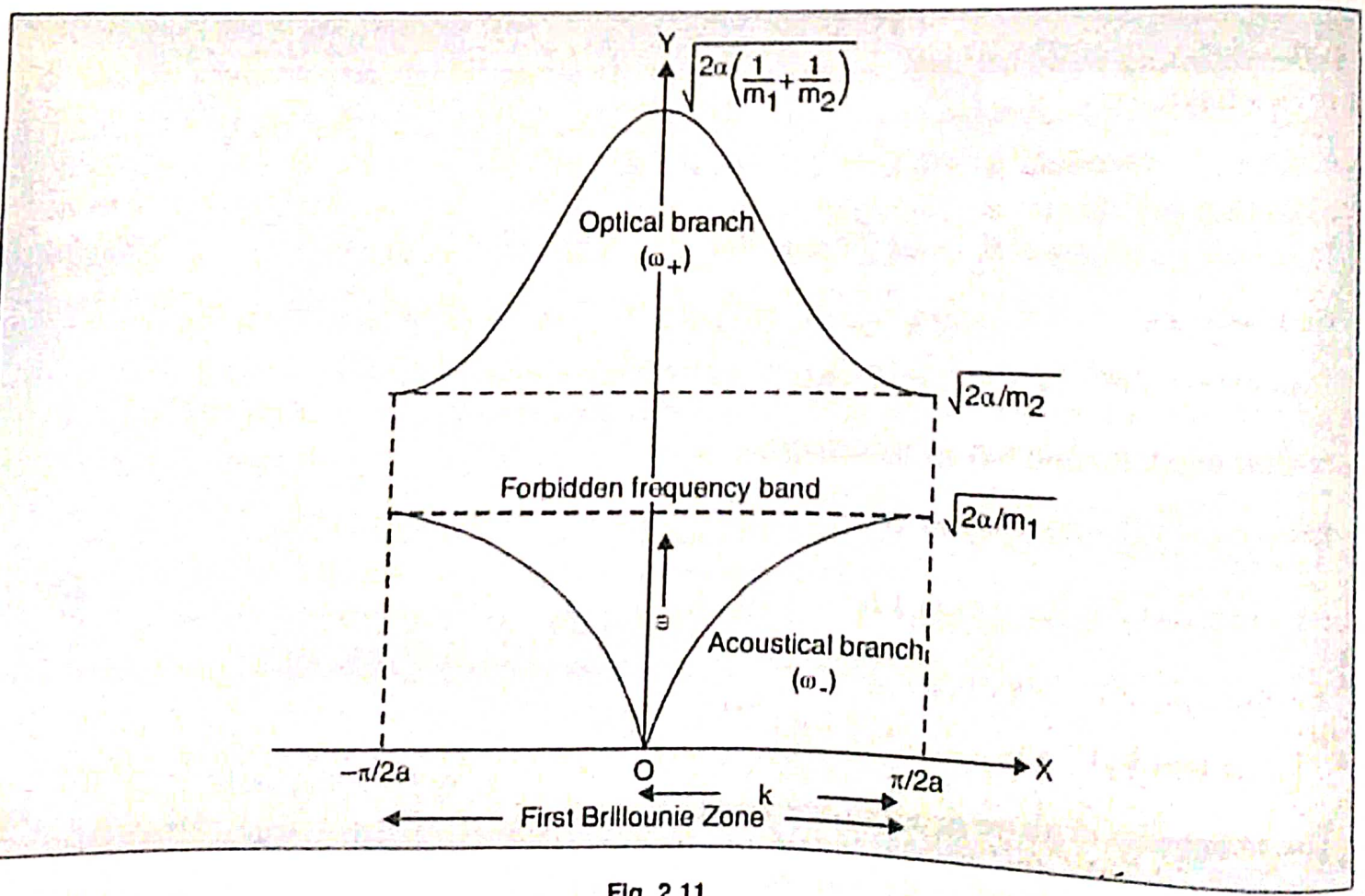


Fig. 2.11

(i) Acoustical branch (Case of ω_-) : The lower branch of dispersion curve in Fig. 2.11 is known as Acoustical curve.

For $k = 0, \sin ka = 0$

hence $\omega_- = 0$

For $ka << 1, \sin ka = ka$

$$\omega_-^2 = \alpha\left(\frac{1}{m_1} + \frac{1}{m_2}\right)$$

In acoustical branch the values of propagation constant k is restricted to the range between $\frac{-\pi}{2a}$ and $\frac{+\pi}{2a}$ as shown in Fig. 2.11.

For $k = \pm \frac{\pi}{2a}$, the frequencies is

$$\omega_- = \sqrt{\frac{2\alpha}{m_1}} \qquad ...(i)$$

The amplitude of vibration for the acoustical branch are equal *i.e.* $A = B$. Here, the types of atoms move in the same direction with the same amplitude as shown in Fig. 2.12 (when $k = 0$).

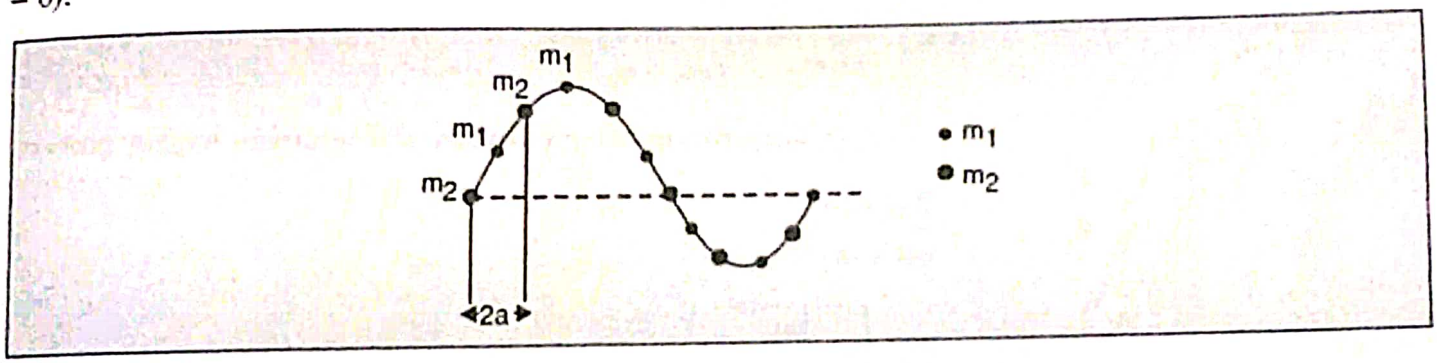


Fig. 2.12

As acoustical branch wave is a travelling wave, the amplitude of vibrations of mass m_2 is zero *i.e.* $B = 0$. The light particles of mass m_1 are all at rest. At the Brillouin zone, the acoustical branch represent standing waves with a phase difference of $\frac{\pi}{2}$ as shown in Fig. 2.13.

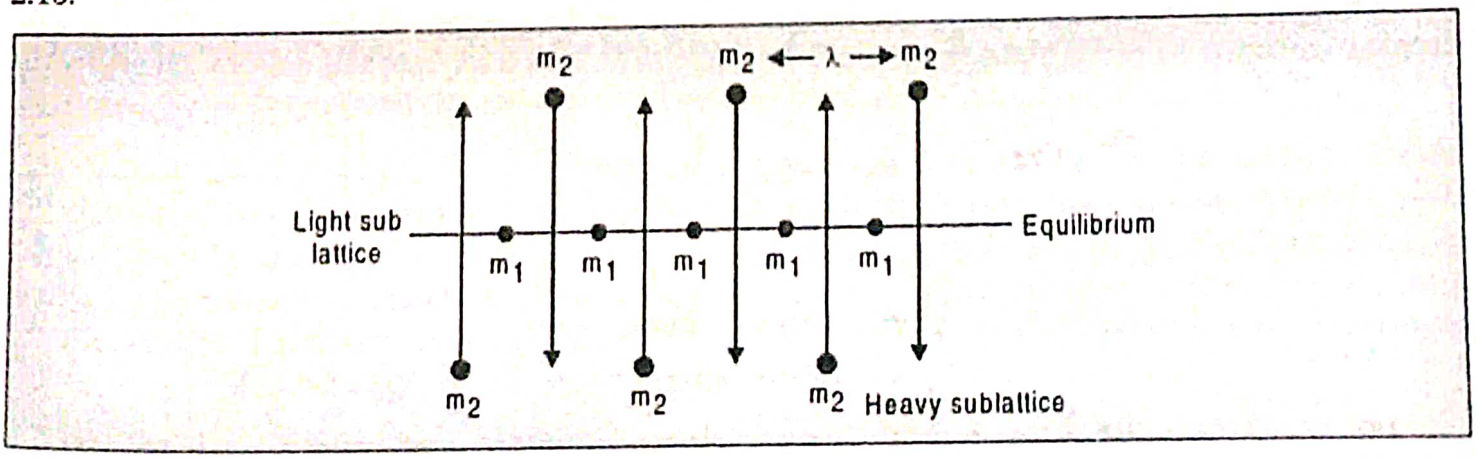


Fig. 2.13

The vibrations in the acoustical branch can be excited by force which compels the atoms in the crystal to move in the same direction. As an example we may force a beam of longitudinal wave such as sound wave to be directed at the surface of a crystal to produce the desired effect. Because of this, the vibrations are termed as the acoustical vibrations and so on dispersion relations, the acoustical branch is constituted.

The acoustical branch vanishes when heavy particle of mass m_2 tends to infinity. When $m_2 \to \infty$, the mid-point between each atom is tied down, thus isolating the atoms from one another. Physically each atom is independent of each other.

The acoustical branch remains unchanged when light particle of mass m_1 tends to zero and the result of monoatomic lattice is obtained.

Derivation of eqn. (i) : The dispersion relation for the acoustical branch is given by the relation

$$\omega_-^2 = \alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right) - \alpha\sqrt{\left(\frac{1}{m}+\frac{1}{m_2}\right)^2 - \frac{4k^2a^2}{m_1m_2}}$$

$$= \alpha\left(\frac{m_1+m_2}{m_1m_2}\right)\left[1-\sqrt{1-\frac{4k^2a^2m_1m_2}{(m_1+m_2)^2}}\right]$$

$$= \alpha\left(\frac{m_1+m_2}{m_1m_2}\right)\frac{2k^2a^2m_1m_2}{(m_1+m_2)^2}$$

(Using Binomial expansion and ignoring higher powers.)

$$= \frac{2\alpha k^2a^2}{(m+m_2)}$$

or $$\omega_- = ka\sqrt{\frac{2\alpha}{(m_1+m_2)}}$$

For long wavelength limits, the dispersion relation reduces to

$$v_p = v_g = a\sqrt{\frac{2\alpha}{(m_1+m_2)}}$$

when $\sin^2 ka = 1$ or $ka = \pm\frac{\pi}{2}$, the ω_- has maximum frequency, so that

$$(\omega_-)^2_{max} = \alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right) - \alpha$$

$$= \sqrt{\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4}{m_1m_2}} = \frac{2\alpha}{m_1}$$

or $$(\omega_-)_{max} = \sqrt{\frac{2\alpha}{m_1}}$$

When the atoms of the lattice vibrate with the same phase and amplitudes about their mean position, the phonons are said to be acoustical phonons. If the displacement is in the direction of the propagation then in some areas the atoms will be closer, and in some areas will be farther apart, as in sound waves in air as shown in Fig. 2.13.

Point to Remember

Acoustic phonons exhibit a linear relationship between frequency and phonon wave vector for long wavelengths. The frequencies of acoustic phonons tend to zero with longer wavelengths.

(ii) Optical branch (Case of ω_+) : The upper branch of the dispersion curve is called optical curve in Fig. 2.11.

For $k \to 0$, $\sin ka \to 0$ *i.e.* it is negligible.

Hence putting $\sin ka = 0$ in dispersion curve relation, we have

$$\omega_+ = \sqrt{2\alpha\left(\frac{1}{m_1} + \frac{1}{m_2}\right)}$$

For $k \to \frac{\pi}{2a}$, $\sin ka \to 1$ and we have

$$\omega_+^2 = \alpha\left(\frac{1}{m_1} + \frac{1}{m_2}\right) + \alpha\sqrt{\left(\frac{1}{m_1} + \frac{1}{m_2}\right)^2 - \frac{4}{m_1 m_2}}$$

$$= \alpha\left(\frac{1}{m_1} + \frac{1}{m_2}\right) + \alpha\left(\frac{1}{m_1} - \frac{1}{m_2}\right)$$

$$\omega_+ = \sqrt{\frac{2\alpha}{m_2}}$$

Hence, the optical branch starts with frequency $\sqrt{2\alpha\left(\frac{1}{m_1} + \frac{1}{m_2}\right)}$ at $k = 0$ and decreases slowly with increase in the value of k and ends with frequency $\sqrt{\frac{2\alpha}{m_2}}$ at $k = \pm\frac{\pi}{2a}$.

The optical branch has the small variation over the entire range of k. Since the modes of the optical branch can be excited with visible light in solids which are partly ionic, we name this branch as the **optical branch**. The ratio of the amplitude (B/A) is negative over the entire range of frequencies by the optical branch.

Optical phonons are out of phase movements of the atoms in the lattice. During vibrations, if one atom moves towards the left then the other atom moves towards right. These phonons are called optical because in most of ionic crystals such as NaCl, phonons are excited by infrared radiation. The electric field component of electromagnetic radiation compels positive sodium ion along the direction of the field and every negative chlorine ion moves in opposite direction to make the crystal vibrate.

At Brillouin zone, the optical phonons have a non-zero frequency. Near the long wavelength limit, optical phonons show no dispersion.

Point to Remember

Optical phonons are responsible for the interactions of a solid with light because they have higher frequencies.

The optical modes are the natural frequency of the light atoms perturbed by the heavy sub-lattice. At $k = \frac{\pi}{2a}$, the heavy sub lattice is not moving as shown in Fig. 2.14.

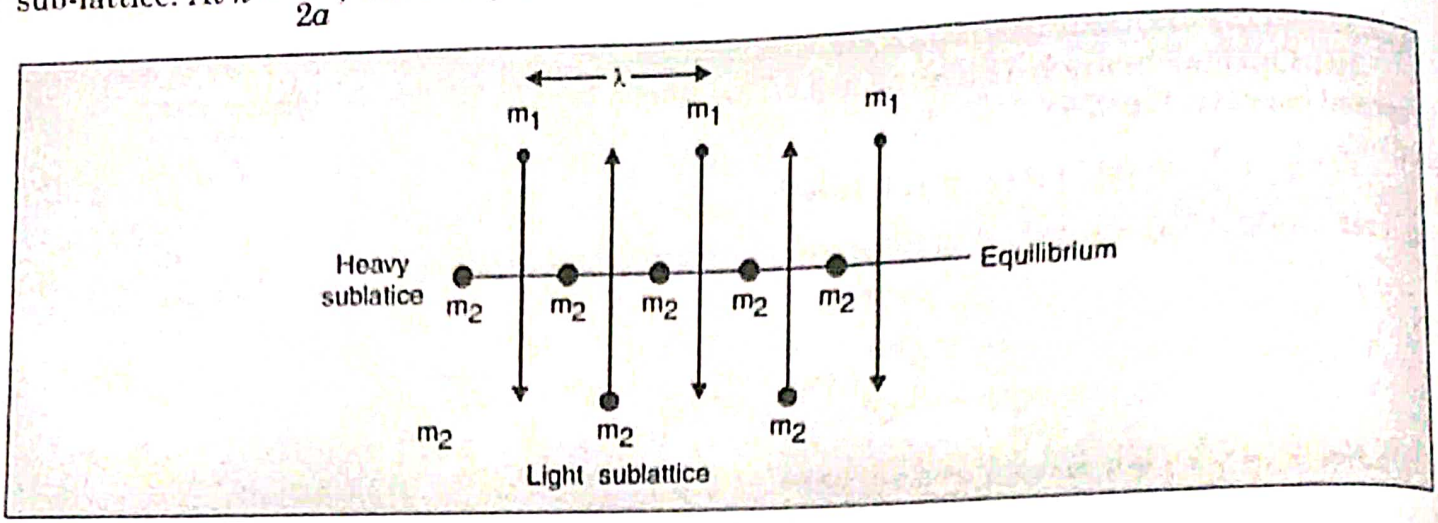


Fig 2.14

The centre of mass of the unit cell remains fixed during the movement of masses, as for the optical branch at $k = 0$, the atoms vibrate in opposite directions as shown in Fig. 2.15.

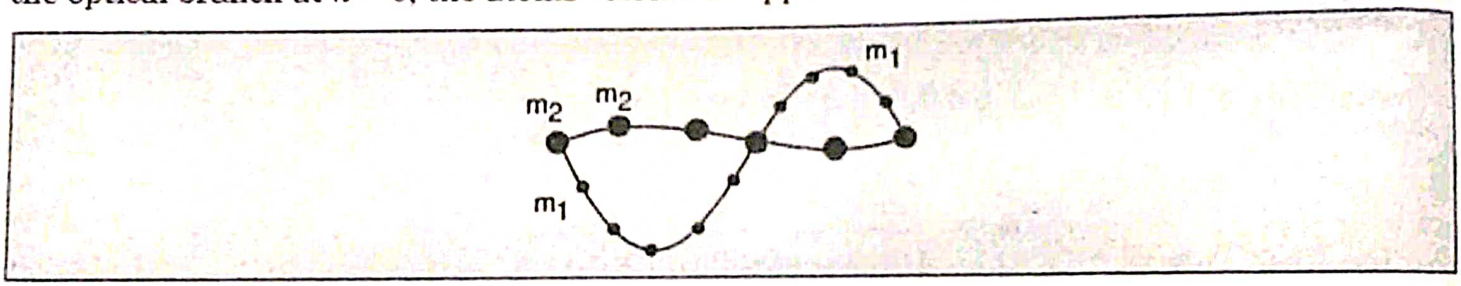


Fig. 2.15

Only the light atoms having mass m_1, vibrate at natural frequency $\sqrt{\frac{2\alpha}{m}}$. The perturbation increases with the decrease in k until at $k = 0$ the two sub lattices are actually vibrating rigidly as shown in Fig. 2.14.

(iii) Forbidden Band : There is a band of frequencies between the two branches – acoustical and optical, which cannot propagate. This band is called Forbidden band. The width of this band depends upon the mass difference of vibrating atoms. If the ratio $\left(\frac{m_2}{m_1}\right)$ is large, then the width of forbidden band is large. But if the two masses are equal *i.e.* $m_1 = m_2$, the gap disappears and the acoustical and optical frequency coincide at $k = \pm \frac{\pi}{2a}$.

2.7 PHONON SPECTRUM IN SOLIDS

We have studied so far that the crystal cannot propagate all the frequencies, they allow only those frequencies which fall in the allowed band. These allowed bands are separated

from each other by forbidden band. If there are N atoms per primitive cell the allowed frequencies split into N-bands.

The field of elastic wave is treated like a gas made up of quanta of the normal modes of the lattice or of phonons having the energy $E = \hbar\omega$ and the momentum of phonons is given by

$$p = \frac{\hbar\omega}{v}$$

where $\vec{v}$ is the velocity of sound. Whenever a crystal is heated, it behaves as a box with phonon gas. Phonons are described by the Bose-Einstein distribution function as photons. The energy density $E(f)$ of electromagnetic radiation consisting of photons lying between frequency f and $f + df$ is given by

$$E(f)\, df = \frac{8\pi h}{c^3} \frac{f^3 df}{e^{\frac{hf}{k_B T}} - 1}$$

where h is Planck's constant, f is frequency, k_B is Boltzmann's constant, c is the velocity of electromagnetic radiation and T is the temperature.

Every oscillating atom represents the normal modes of the lattice in which all the atoms of the crystal take part vibrating with the same frequency ω.

The energy of a quantum oscillator is expressed as

$$E_n = \left(n \pm \frac{1}{2}\right) \hbar\omega$$

where $n = 0, 1, 2, \ldots\ldots$ is the quantum number. Fig. 2.16 shows the energy spectrum of a linear harmonic oscillator. It consists of a set of discrete levels spaced at the interval of $\hbar\omega$.

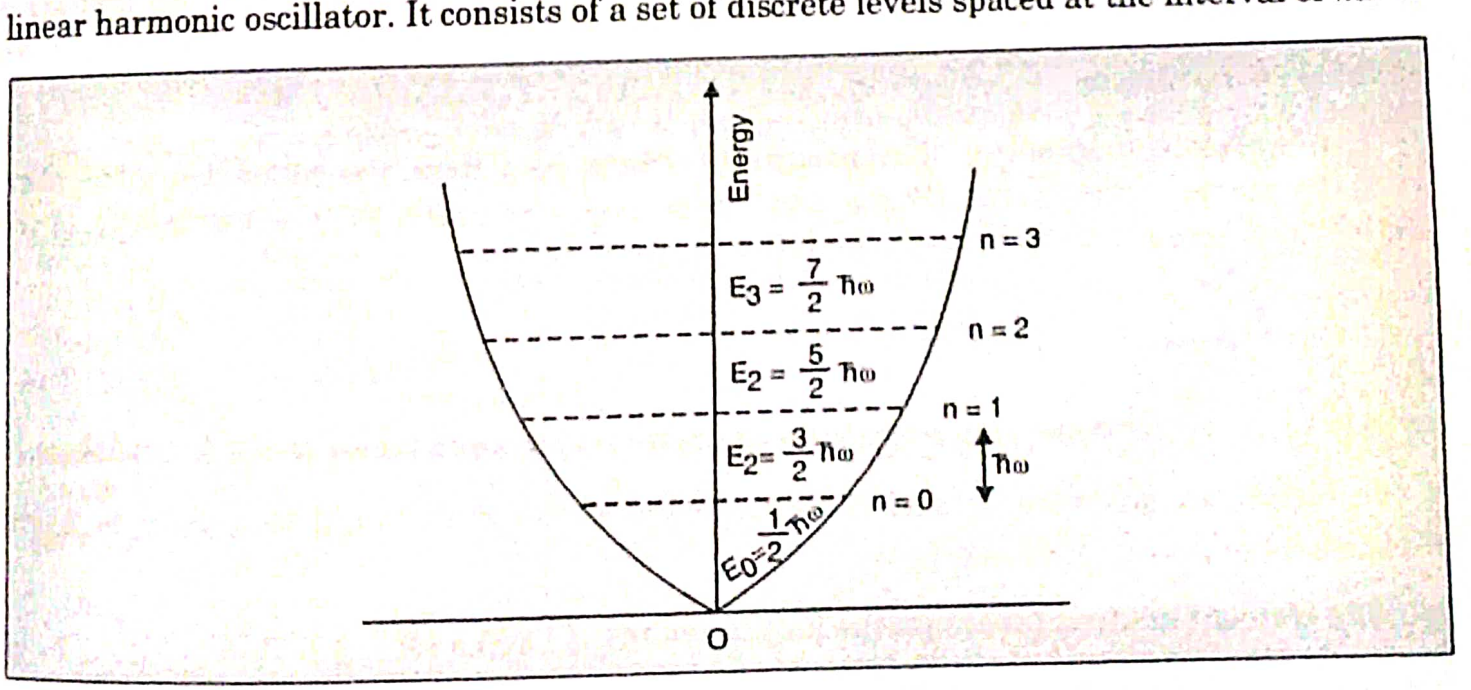


Fig. 2.16

The minimum portion of energy that can be absorbed or emitted by the lattice in the process of thermal vibrations corresponds to the transition of the normal mode being excited

from the given energy level to the adjacent level and is equal to $E = \hbar\omega$. Depending on the intensity of excitation of the normal mode, the crystal can emit a definite number of phonons. Hence, if some mode is excited to the third level in Fig. 2.16, the energy becomes $\frac{7}{2}\hbar\omega$. It means that the normal mode has produced three identical phonons each with an energy of $\hbar\omega$. The graph between energy density $E(f)$ and the energy E is shown in Fig. 2.17.

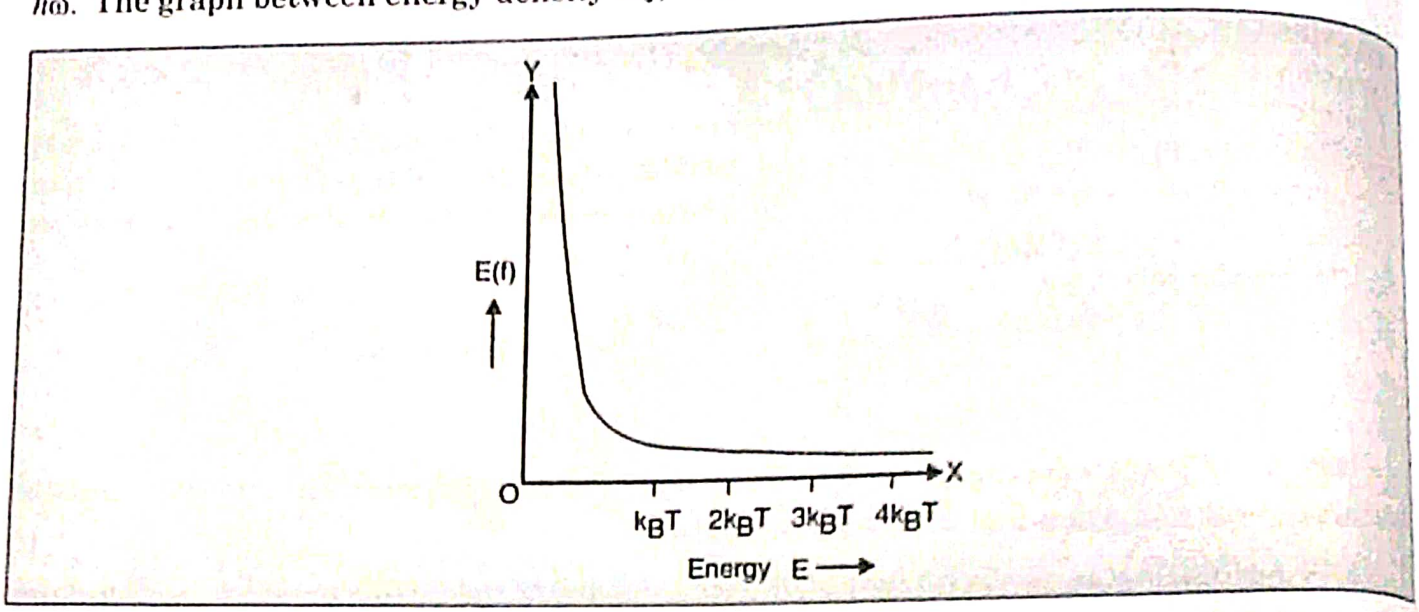


Fig. 2.17

The vibration spectrum of the phonon waves occupy a wide range of frequency from 10^{10} Hz to 10^{13} Hz. Although there is no direct proof that the energy of an elastic wave is quantised, but experimentally it is proved that phonon do exist. The proofs are

(i) Inelastic scattering of X-rays by phonon : A phonon is created or absorbed in the umklapp process in which the phonon spectrum of solids can be inelastic diffused scattering of X-ray photons. In this experiment we find the phonon frequency as a function of the wave vector $\vec{k}$ of the phonon.

(ii) Inelastic scattering of neutrons by Phonons : Here, the scattering takes place from the nuclei of the atoms. The general wave vector equation for the kinematics of the scattering of neutron beam by a crystal lattice is given by

$$\vec{k} = \vec{k}' + \vec{G} + \vec{k}_i$$

where $\vec{k}'$ is the wave vector of scattered photon, $\vec{k}$ is wave vector of incident photon, $\vec{G}$ is the reciprocal lattice vector and $\vec{k}_i$ is the wave vector of a created phonon or $\vec{k}_i$ is the wave vector of phonon absorbed in the process.

The incident neutron possesses the kinetic energy (E) given by

$$E = \frac{1}{2} m_n v^2$$

where m_n is the mass of the neutron and $\vec{v}$ is the velocity.

or $$E = \frac{1}{2}\frac{p^2}{m_n}$$

$$= \frac{h^2k^2}{2m_n} \qquad (\because \text{ the momentum } \vec{p} = h\vec{k})$$

Here $\vec{k}$ is the wave vector the neutron. Let $\vec{k}'$ be the wave vector of the scattered neutron, then its kinetic energy is given by

$$E' = \frac{1}{2}\frac{h^2\vec{k}'^2}{m_n}$$

Using the principle of conservation of kinetic energy, we have

$$E = E'$$

or $$\frac{h^2\vec{k}^2}{2m_n} = \frac{h^2\vec{k}'^2}{2m_n} \pm h\Omega s$$

where Ω is the angular frequency of phonon of wave vector k and $h\Omega$ is the kinetic energy of the phonon created or absorbed.

It is essential to obtain the energy gain or loss of the scattered neutron as a function of the scattering direction $(k - k')$ so as to obtain dispersion relation. A schematic diagram of an inelastic neutron scattering apparatus is shown in Fig. 2.18.

Time of Flight Method : This is a general method for calculating the kinetic energy of a travelling neutron by measuring the time between the two fixed points where the distance is known.

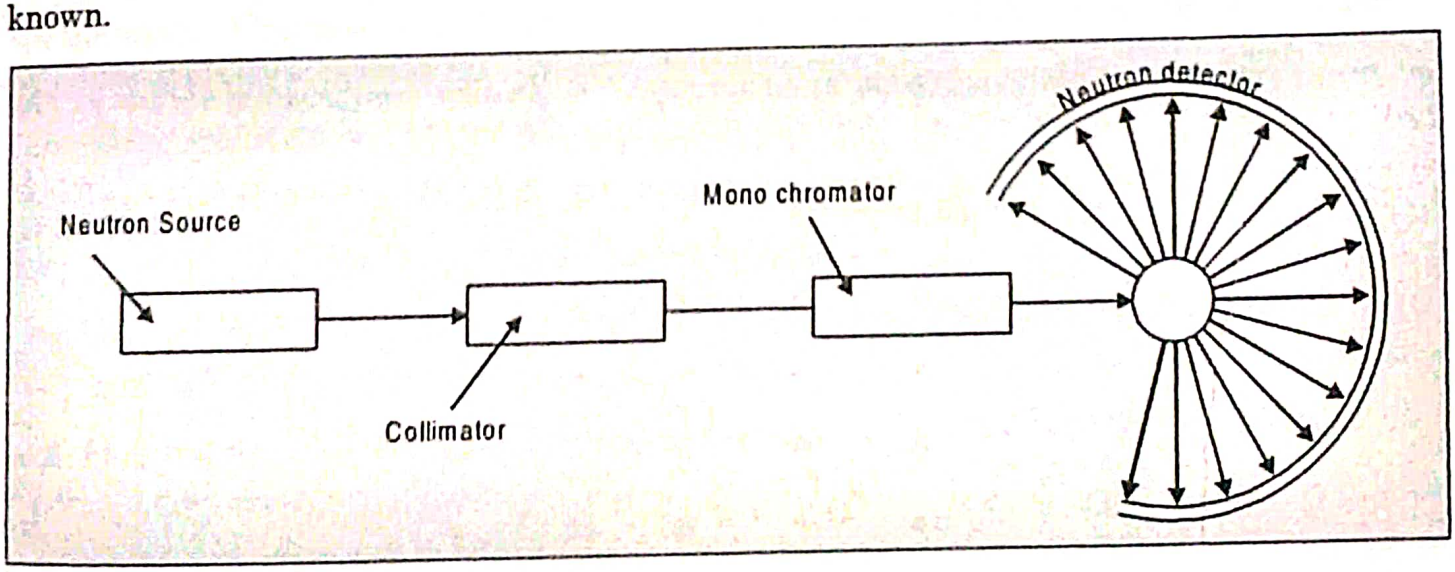


Fig. 2.18

A monoenergetic beam of neutrons having to kinetic energy equal to $h^2k^2/2m_n$ and of wavevector k is allowed to hit the crystal from a collimator. The beam gets scattered in different directions corresponding to the spectrum of possible $\vec{k}_i$ vectors of lattice vibrations.

The scattered neutrons are detected by the neutron detectors which are placed at all angles surrounding the crystal as shown in Fig. 2.18. After detecting the neutrons, the detectors calculate the time of flight. The kinetic energy of the scattered photon is obtained by the time of flight. The angle through which neutron scatters gives the value of $\vec{k}'$, the momentum of the scattered neutron.

Point to Remember

In 1935, only three years after the discovery of the neutron by Chadwick, a pair of rotating disc was used to prove that the slow neutrons are in thermal velocity range.

Fig. 2.19 shows the graph between the scattering angle and the intensity, determines the reciprocal lattice, vector G. The peak in the graph occurs at Bragg's angle.

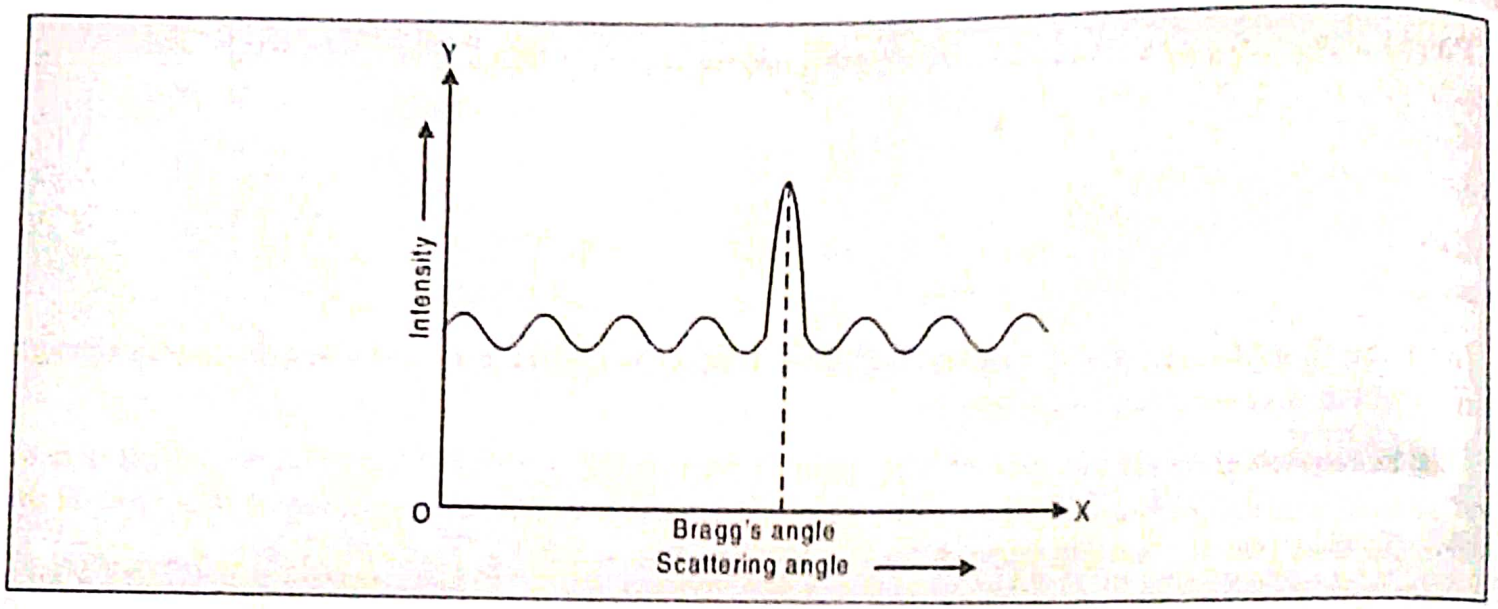


Fig. 2.19

The wavevector K_f for a phonon which is created or absorbed is obtained by knowing the reciprocal vector $\vec{G}$. This is achieved by using modified Ewald's construction shown in Fig. 2.20.

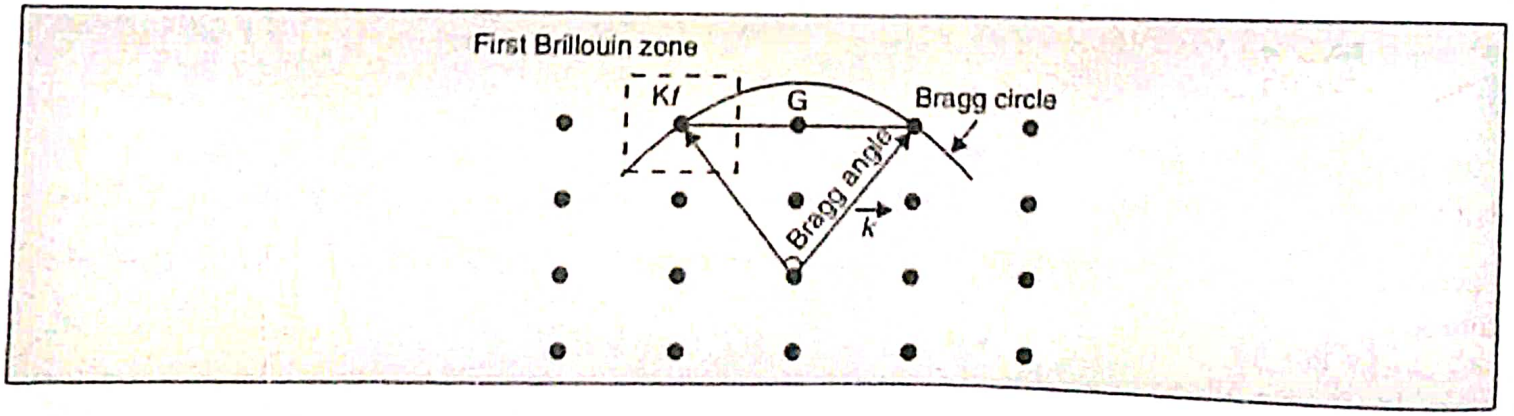


Fig. 2.20

The dispersion curves of sodium for phonons propagating in (1 0 0), (1 1 0) and (1 1 1) directions are shown in Fig. 2.21, both for transverse and longitudinal wave at a fixed temperature of 90K.

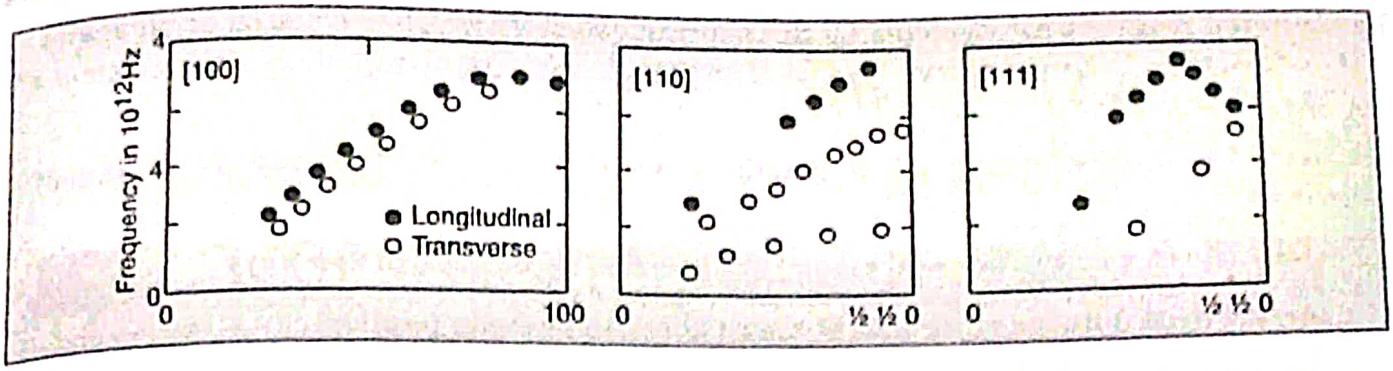


Fig. 2.21.

2.8 DULONG AND PETIT'S LAW

Pierre Louis Dulong (1785 – 1838) and Alexis Therese Petit (1791 – 1820), the two French physicists are known for Dulong and Petit's law concerning specific heat of metals which they formulated in 1819. Let us first summarise the concepts of classical theory of lattice vibration and heat capacity.

(*i*) We assume atoms in a solid to vibrate freely about their mean equilibrium position in the same way as the harmonic oscillator in three dimensional space vibrates.

(*ii*) Degree of freedom of a system is the number of independent parameters required to define its state e.g. a free particle in the space has three degrees of freedom because the position of the particle can be specified by three position coordinates.

(*iii*) Molar specific heat at constant pressure is given as

$$C_p = \left(\frac{dQ}{dT}\right)_p$$

where dQ is the amount of heat energy required to raise the temperature of unit mass of substance through dT keeping the pressure constant.

(*iv*) Molar specific heat at constant volume is given by

$$C_v = \left(\frac{dQ}{dT}\right)$$

(*v*) In solids the two specific heats do not differ much at low temperature. Therefore by specific heat of a solid we mean specific heat at constant volume.

(*vi*) At constant volume $dV = 0$, so the expression for the first law of thermodynamics becomes

$$dQ = dU + PdV$$

or

$$dQ = dU$$

where dU is the change in internal energy. Hence

$$C_V = \left(\frac{dQ}{dT}\right)_V$$

$$= \left(\frac{dU}{dT}\right)_V \qquad \ldots(1)$$

(*vii*) The internal energy dU is largely contributed due to vibrational energy of atomic oscillators.

(*viii*) The increase in internal energy dU in solids takes place in two ways.

(*a*) due to continuous vibrations of atoms about their mean position.

(*b*) due to thermal excitation of electrons to higher energy states as in metals.

(*ix*) The net internal energy U is given as

$$U = U_{\text{lattice}} + U_{\text{elec}}$$

and correspondingly, we obtain,

$$C_V = \left(\frac{dU}{dT}\right)_V$$

$$= \left[\frac{d}{dT}(U_{\text{lattice}} + U_{\text{elec}})\right]_V$$

$$= \frac{d}{dT}(U_{\text{lattice}}) + \frac{d}{dT}(U_{\text{elec}})$$

$$= C_{\text{lattice}} + C_{\text{elect}}$$

where C_{lattice} is known as lattice specific heat or lattice heat capacity. Here we use the term heat capacity instead of lattice heat capacity.

(*x*) The atomic oscillators vibrate with the same frequency but their energies are different as they vibrate with different amplitudes.

(*xi*) The atomic oscillator takes up continuum of energy values from zero to infinity.

(*xii*) The total energy of solid at a given temperature is N times the average energy of the oscillator.

Let us derive an expression for the energy U of a three dimensional harmonic oscillator of mass m and angular frequency ω

$$U = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2$$

$$= \frac{p^2}{2m} + \frac{1}{2}m\omega^2(x^2 + y^2 + z^2) \qquad (\because r^2 = x^2 + y^2 + z^2)$$

where $\vec{p}$ is the momentum and $\vec{r}$ is the displacement from the mean position.

Applying Boltzmann's distribution law, the average energy of each harmonic oscillator is given by

$$\overline{U} = \frac{\int U\, e^{-[U/k_BT]}\, dU}{\int e^{-U/k_BT}\, dU}$$

Here k_B is the Boltzmann's constant. Substituting the value of U, we have,

$$\overline{U} = \frac{\iint_{p\,r} \left(\frac{p^2}{2m} + \frac{1}{2} m\omega^2 r^2\right) e^{-p^2/2\,mk_BT}\, e^{-\frac{m\omega^2 r^2}{2k_BT}}\, dpdr}{\iint_{p\,r} e^{\frac{-p^2}{2\,mk_BT}}\, e^{-\frac{m\omega^2 r^2}{2k_BT}}\, dpdr}$$

$$\overline{U} = \frac{\iint_{p\,r} \frac{p^2}{2m}\, e^{-\frac{p^2}{2\,mk_BT}}\, e^{-\frac{m\omega^2 r^2}{2k_BT}}\, dpdr}{\iint_{p\,r} e^{\frac{-p^2}{2\,mk_BT}}\, e^{-\frac{m\omega^2 r^2}{2k_BT}}\, dpdr}$$

$$+ \frac{\iint_{p\,r} \frac{1}{2} m\omega^2 r^2\, e^{-\frac{p^2}{2\,mk_BT}}\, e^{-\frac{m\omega^2 r^2}{2k_BT}}\, dpdr}{\iint_{p\,r} e^{\frac{-p^2}{2\,mk_BT}}\, e^{-\frac{m\omega^2 r^2}{2k_BT}}\, dpdr}$$

$$= \frac{\int_{-\infty}^{\infty} \frac{p^2}{2m}\, e^{-\frac{p^2}{2\,mk_BT}}\, dp}{\int_{-\infty}^{+\infty} e^{-\frac{p^2}{2\,mk_BT}}\, dp} + \frac{\int_{-\infty}^{\infty} \frac{m\omega^2 r^2}{2}\, e^{-\frac{m\omega^2 r^2}{2k_BT}}\, dr}{\int_{-\infty}^{\infty} e^{-\frac{m\omega^2 r^2}{2k_BT}}\, dr}$$

Let $$\frac{p^2}{2\,mk_BT} = A^2 \text{ (say)}$$

and $$\frac{m\omega^2 r^2}{2k_BT} = B^2$$

So, we get

$$\overline{U} = \frac{k_BT \int_{-\infty}^{\infty} A^2\, e^{-A^2}\, dA}{\int_{-\infty}^{\infty} e^{-\alpha^2}\, dA} + \frac{k_BT \int_{-\infty}^{\infty} B^2\, e^{-B^2}\, dB}{\int_{-\infty}^{\infty} e^{-B}\, dB}$$

Using standard integrals

$$\int_{-\infty}^{\infty} A^2 e^{-A^2} dA = \sqrt{\frac{\pi}{2}}$$

and $\int_{-\infty}^{\infty} e^{-A^2} dA = \sqrt{\pi}$, we have

$$\bar{U} = \frac{k_B T \sqrt{\frac{\pi}{2}}}{\sqrt{\pi}} + \frac{k_B T \sqrt{\frac{\pi}{2}}}{\sqrt{\pi}}$$

$$= \frac{k_B T}{2} + \frac{k_B T}{2} = k_B T$$

Therefore, the net vibrational energy of a crystal having N identical harmonic oscillators in three dimensions is given by

$$U = 3N(\bar{U})$$

$$= 3N k_B T$$

where N is Avogadro's constant.

Using equation (*), the molar heat capacity at constant volume is given by

$$C_V = \left(\frac{dU}{dT}\right)_{V = \text{constant}}$$

$$= \frac{d}{dT}[3Nk_B T] = 3Nk_B$$

$$\therefore \quad C_V = 3R \qquad (\because Nk_B = R)$$

The above statement is referred as Dulong and Petit's law which states that the specific heat of all solids at all temperatures is constant and is equal to $3R$. The specific heat is independent of temperature and nature of solid.

We know that universal gas constant $R = 8.31\ J\ mole^{-1}\ K^{-1}$

$$\therefore \quad C_V = 3R$$

$$= 3 \times 8.31$$

$$\simeq 25\ J\ mole^{-1}\ K^{-1}$$

The Result : Dulong and Petit's law is in agreement with the experimental observations for many solids only at high temperatures. According to this law at high temperatures, the specific heat of a solid is independent of temperature. The law also confirms that the specific heat is constant.

Point to Remember

Surprisingly, Dulong and Petit were unaware of the relationship with gas constant R since during their times in 1819 the gas constant had not yet been defined from kinetic theory of gases.

Dulong and Petit simply found that the value of specific heat of a solid per mole was about 25 JK^{-1} which is same as 3R.

Limitations of Dulong-Petit's Law

- Dulong and Petit's law fails for light elements such as boron, beryllium and carbon (or diamond). Experimentally, it has been found that the value of Cv for light elements is much lower than the constant value of 25 $J\,K^{-1}\,mole^{-1}$.
- Dulong and Petit's law fails to keep the specific heat of solids at low temperatures.
- The value of Cv approaches zero as temperature T approaches zero kelvin.
- The experimental results shows how Cv varies with temperature for several elements (Fig. 2.22).

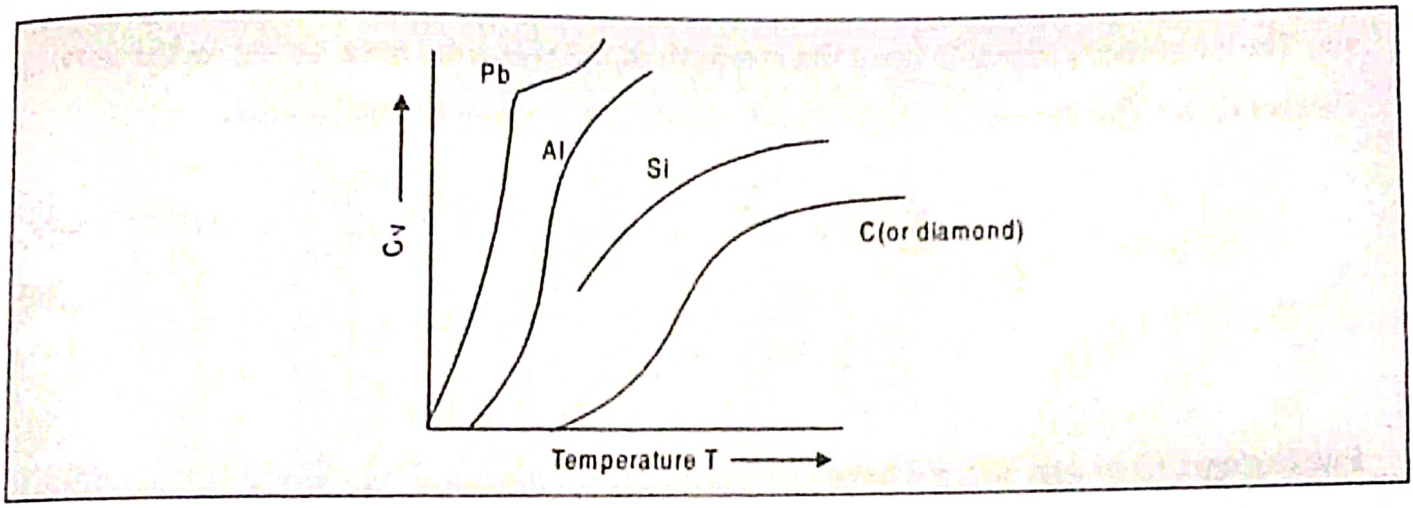


Fig. 2.22

- Einstein observed that Dulong and Petit's law fails badly for diamond.

2.9 EINSTEIN THEORY OF SPECIFIC HEAT

The discrepancies in Dulong and Petit's law of specific heat were removed by Albert Einstein (1879 – 1955), a German born physicist by the application of quantum theory. In his theory of specific heat, Einstein assumed that

(*i*) All atoms are identical independent simple harmonic oscillators, vibrating with the same natural frequency.

(*ii*) Every crystalline solid consists of N atoms, each atom is equivalent to three mutually perpendicular Planck oscillators. A Planck oscillator is an oscillator which can absorb or emit energy in amounts which are integral multiples of Planck's constant h times the frequency of the oscillator and follows the Planck's law for the black body radiation on the basis of Bose-Einstein's statistics.

(*iii*) The energy spectrum of Planck oscillator is discontinuous as assumed in Dulong Petit's law but has discrete values in accordance with quantum theory.

(*iv*) Each of $3N$ harmonic oscillator have the quantised energy.

$$U_n = \left(n + \frac{1}{2}\right) hf \qquad \ldots(i)$$

where $n = 0, 1, 2, \ldots\ldots$, h is Planck's constant and f is the frequency.

Point to Remember

Originally, Einstein used the Planck's result $U_n = nhf$ rather than the wave mechanical result as given in assumption (*iv*) for the energy levels of an *harmonic oscillator*.

(*v*) Instead of classical law of equipartition that is $\frac{1}{2} k_B T$ for each degree of freedom, Einstein assumed the mean energy of Planck's oscillator for each degree of freedom *i.e.*

$$\overline{U} = \frac{hf}{\frac{hf}{e^{k_B T} - 1}}$$

(*vi*) The frequency f depends upon the strength of the restoring force acting on the atom.

Derivation : The average energy of such oscillators is given by the relation

$$\overline{U} = \frac{\sum_{n=0}^{\infty} U_n e^{-\frac{U_n}{k_B T}}}{\sum_{n=0}^{\infty} e^{-\frac{U_n}{k_B T}}} \qquad \ldots(ii)$$

Putting eqn. (*i*) in eqn. (*ii*), we have

$$\overline{U} = \frac{\sum_{n=0}^{\infty} \left(n + \frac{1}{2}\right) hf \, e^{\left[\frac{-\left(n + \frac{1}{2}\right) hf}{k_B T}\right]}}{\sum_{n=0}^{\infty} e^{-\left[\frac{\left(n + \frac{1}{2}\right) hf}{k_B T}\right]}}$$

Substitute $\frac{-hf}{k_B T} = x$ (say), so that,

$$\overline{U} = \frac{hf \sum_{n=0}^{\infty} \left(n + \frac{1}{2}\right) e^{\left(n + \frac{1}{2}\right) x}}{\sum_{n=0}^{\infty} e^{\left(n + \frac{1}{2}\right) x}}$$

$$\overline{U} = \frac{hf\left[\frac{1}{2}e^{x/2} + \frac{3}{2}e^{3x/2} + \frac{5}{2}e^{5x/2} + ...\right]}{\left[e^{x/2} + e^{3x/2} + e^{5x/2} + ...\right]}$$

$$= hf\frac{d}{dx}\left\{\log_e\left[e^{x/2} + e^{3x/2} + e^{5x/2} + ...\right]\right\}$$

$$= hf\frac{d}{dx}\left[\log_e e^{x/2}\left[1 + e^x + e^{2x} + ...\right]\right]$$

$$= hf\frac{d}{dx}\left[\log_e e^{x/2} + \log_e (1 + e^x + e^{2x} + ...)\right]$$

$$= hf\frac{d}{dx}\left[\frac{x}{2} - \log_e (1 - e^x)\right]$$

$$[\because \log (1 + e^x + e^{2x} + ...) = -\log(1 - e^x)]$$

$$= hf\left[\frac{1}{2} + \frac{e^x}{(1 - e^x)}\right] = hf\left[\frac{1}{2} + \frac{1}{(e^{-x} - 1)}\right]$$

Substituting $x = \frac{-hf}{k_B T}$, we have,

$$\overline{U} = hf\left[\frac{1}{2} + \frac{1}{[e^{hf/k_B T} - 1]}\right]$$

or

$$\overline{U} = \frac{1}{2}hf + \frac{hf}{[e^{hf/k_B T} - 1]}$$

The first term on the right hand side of above equation is referred as zero point energy. This energy is not dependent on temperature. This confirms that the vibrational energy is not zero even if the temperature is reduced to zero kelvin.

If N is the number of atoms in the crystal then it is equivalent to $3N$ oscillators, so that the total internal energy becomes

$$U = 3N\overline{U}$$

$$= 3N\left[\frac{1}{2}hf + \frac{hf}{\left[e^{hf/k_B T} - 1\right]}\right]$$

$$= \frac{3Nhf}{2} + \frac{3Nhf}{\left[e^{\frac{hf}{k_B T}} - 1\right]}$$

By definition, the heat capacity (or the specific heat at constant volume) Cv is defined as

the amount of heat required to increase the temperature of the crystal by unit temperature at constant volume *i.e.*

$$C_V = \left(\frac{dU}{dT}\right)_V$$

$$= \frac{d}{dT}\left[\frac{3Nhf}{2} + \frac{3Nhf}{\left[e^{\frac{hf}{k_BT}} - 1\right]}\right]$$

$$= 0 + \frac{d}{dT}\left[\frac{3Nhf}{\left[e^{\frac{hf}{k_BT}} - 1\right]}\right]$$

$$= 3Nhf\left[\frac{e^{\frac{hf}{k_BT}} \cdot \frac{d}{dT}[3Nhf] - e^{\frac{hf}{k_BT}}\left[\frac{-hf}{k_BT^2}\right]}{\left[e^{\frac{hf}{k_BT}} - 1\right]^2}\right]$$

$$\left[\because \frac{d}{dT}(3Nhf) = 0\right]$$

$$= 3Nk_B\left(\frac{hf}{k_BT}\right)^2 \frac{e^{\frac{hf}{k_BT}}}{\left[e^{\frac{hf}{k_BT}} - 1\right]^2}$$

Putting $hf = \theta_E k_B$

where θ_E is called Einstein's temperature. Now the expression for total specific heat of a solid can be written as

$$C_V = 3Nk_B\left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{\left[e^{\theta_E/T} - 1\right]^2}$$

Special Cases : Let us now examine the behavior of specific heat in extreme temperature limits.

(i) At very high temperature : When the temperature is very high, *i.e.*

$T >> \theta_E$, then

$$\left(\frac{\theta_E}{T}\right) << 1$$

So, $$e^{\theta_E/T} = 1 + \frac{\theta_E}{T} + \frac{1}{2}\left(\frac{\theta_E}{T}\right)^2 + \ldots\ldots$$

$$= 1 + \frac{\theta_E}{T}$$ (neglecting higher order terms)

Therefore, $$C_V = 3Nk_B \left(\frac{\theta_E}{T}\right)^2 \frac{[1 + \theta_E/T]}{\left(\frac{\theta_E}{T}\right)^2}$$

$$= 3Nk_B + 3Nk_B \left(\frac{\theta_E}{T}\right)$$

When $T \longrightarrow \infty$, then $\left(\frac{\theta_E}{T}\right) \longrightarrow 0$

Hence, $$C_V = 3\,N\,k_B$$

$$= 3R \qquad (\because\ Nk_B = R)$$

This result is same as Dulong and Petit's law which confirms that specific heat of solids is independent of temperature. Thus Einstein's theory on specific heat is satisfactory at the high temperature limit because the quantum aspects become irrelevant.

(ii) At low temperatures : When $T << \theta_E$ then

$e^{hf/k_BT} >> 1$, so that

$e^{\theta_E/k_BT} = [1 - e^{\theta_E/T}]$

So that the expression for C_V becomes

$$C_V = 3Nk_B \left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{e^{2\theta_E/T}}$$

$$= 3R \left(\frac{\theta_E}{T}\right)^2 e^{-\theta_E/T}$$

When temperature T approaches zero, the exponential term $e^{-\theta_E/T}$ approaches zero. Therefore the specific heat C_V approaches zero.

Results : Einstein's theory of specific heat matches with experimental facts at high as well as at low temperatures.

At high temperatures, the oscillator is fully, excited, acquiring an average energy equal to k_BT which leads to a molar specific heat $C_V = 3R$.

At low temperatures, the oscillator is essentially unexcited, and hence $C_V = 0$. In simple words, the oscillator is frozen in its ground state. This freezing explains the reason why the vibrational modes in diatomic molecules, such as hydrogen, do not contribute to specific heat, except at high temperatures.

Fig. 2.23 shows the graphical comparison of the experimental value of the heat capacity

for diamond shown with dots with values calculated on Einstein's theory shown by a line using Einstein's temperature $\theta_E = 1320\ K$.

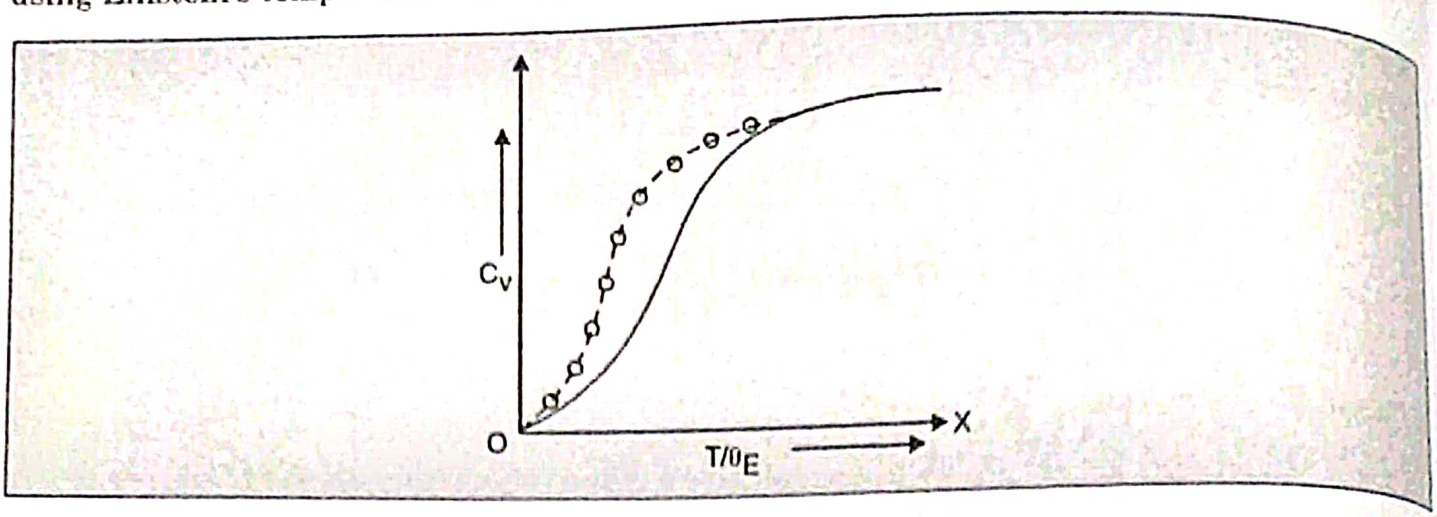


Fig. 2.23

Thus, the Einstein's theory gave a better explanation of the behaviour of specific heat C_V with the temperature as compared with Dulong and Petit's law.

Limitations : Einstein's theory fails to explain the low temperature behaviour of specific heat of solids.

Experimentally, $C_V \propto T^3$ whereas Einstein's theory predicts that $C_V \propto e^{-\theta_E/T}$. The reason for this flaw is because the Einstein's theory is an oversimplified one.

In reality, the atoms forming harmonic oscillators are coupled together with wide range of frequencies. So the assumption that all atoms oscillate independently of each other seems to be not valid.

2.10 DEBYE THEORY OF SPECIFIC HEAT

Debye theory was developed by Peter Debye (1884 – 1966) a Dutch-American physicist, in 1912 for estimating the phonon contribution to the specific heat in a solid. The theory regards the vibrations of the atomic lattice as phonons in a box. This is contrary to Einstein's theory which regards the solid as many individual, non-interacting quantum harmonic oscillators. This Debye theory also corrects the failures of Einstein's theory by predicting the low temperature dependence of the specific heat. Debye insisted that the crystal vibrates in number of modes with crystal as a continuous media.

In his theory Debye assumed that

(i) Solid is treated as an isotropic continuous elastic media in which the motion of each atom is influenced by its neighbours.

(ii) Solid is non-dispersive which means that the velocity of sound is not dependent on frequency.

(iii) Solid vibrates as a whole having frequency range from acoustic to infrared regions.

(iv) The internal energy of the crystal is due to the vibrations of individual atoms present in the elastic stationary waves caused by the vibrations of individual atoms.

(v) The energy of elastic stationary waves is quantised. A quantum of vibrational energy, called phonon has an energy hf similar to that of a photon where f is the frequency of vibration.

Derivation : A solid state equivalent of Planck's law of black body radiation is the Debye model. In Planck's law, the electromagnetic radiation is considered as a gas of photons in a box whereas in Debye model the vibrations of atoms in a solid are considered as phonons in a box.

Let us consider a cube of side L. If both the ends of the side of cube are fixed, then the resultant wave has a displacement given by

$$y = -2a \cos \frac{2\pi v_n t}{\lambda_n} \sin \frac{2\pi}{\lambda_n} x$$

$$= A \cos \frac{2\pi v_n t}{\lambda_n} \qquad \ldots(i)$$

where A is the amplitude of the resultant pulse which varies with distance x from the origin, a is the amplitude of vibrating atom, v_n is the velocity of wave for nth atom, λ_n is the wavelength and t is the time. The resultant displacement y shows that there is no propagation of resultant displacement and so the wave represented by equation (i) is a stationary wave.

At one end of side of a cube, $x = 0$ so that equation (i) can be written as

$$y = -2a \cos \frac{2\pi v_n t}{\lambda_n} \sin (0)$$

$$= (0) \qquad (\because \sin 0° = 0)$$

At the other end of side of a cube, we have

$$x = L$$

So eqn. (i) can be written as

$$y = -2a \cos \frac{2\pi v_n t}{\lambda_n} \sin \frac{2\pi L}{\lambda_n}$$

At the fixed end $y = 0$

$$\therefore 2a \cos \frac{2\pi v_n t}{\lambda_n} \sin \frac{2\pi L}{\lambda_n} = 0$$

or $$\sin \frac{2\pi L}{\lambda_n} = 0 \qquad \left(\because 2a \cos \frac{2\pi v_n t}{\lambda_n} \neq 0\right)$$

$$= \sin 0, \sin \pi, \sin 2\pi, \ldots..$$

$$\sin \frac{2\pi L}{\lambda_n} = \sin n\pi \qquad \text{where } n = 0, 1, 2, 3, \ldots..$$

$$\frac{2\pi L}{\lambda_n} = n\pi$$

$$\frac{2L}{\lambda_n} = n$$

Hence the wavelength of the resonating modes of the sonic disturbances inside the cube is given as

$$\lambda = \frac{2L}{n}$$

when $n = 1$, the first normal mode of vibration of stationary waves set up along the side of a cube is given by wavelength λ_1

$$\lambda_1 = \frac{2L}{1}$$

or $$L = \frac{\lambda_1}{2}$$

The side of a cube vibrates as a whole in one segment as shown in Fig. 2.24.

The energy of a phonon is

$$E_n = h f_n$$

where f_n is the frequency of the phonon.

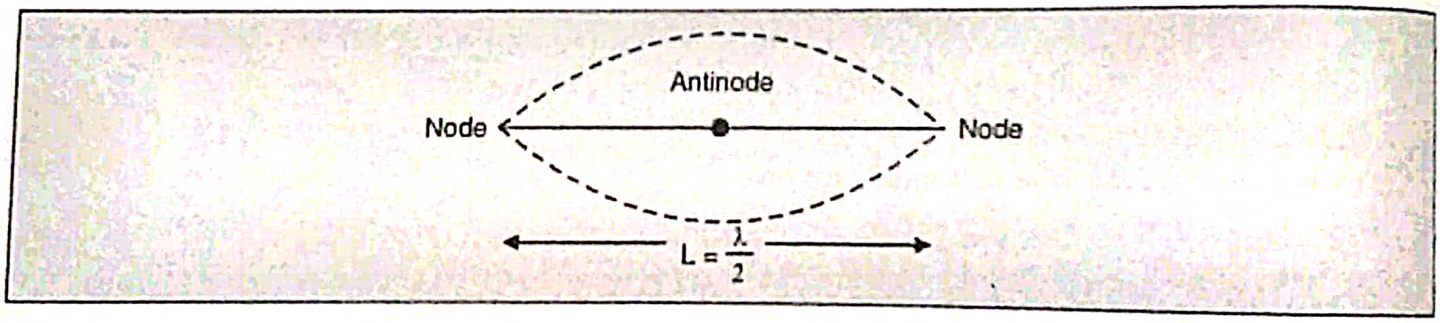


Fig. 2.24.

or $$E_n = \frac{h v_n}{\lambda_n} = \frac{h v_n n}{LL} \qquad \left(\because \lambda_n = \frac{2L}{n}\right)$$

where v_n is the velocity of sound inside the solid in three dimensions and f_n is the frequency of the phonon.

$$E_n^2 = p_n^2 v_n^2$$

$$= \left(\frac{h v_n}{2L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

where p is the momentum of the phonon and n_x, n_y and n_z are the quantum numbers which are positive integers.

Let us now calculate the expression for the total energy U in the cube

$$U = \sum_n E_n \overline{N}(E_n)$$

where $\overline{N}(E_n)$ is the number of phonons in the cube of side L with energy E_n. Mathematically, the total energy is the sum of energy multiplied by the number of phonons with energy.

Now here lies the difference between the Debye theory and Planck's law of black body radiations. Here, in Debye theory, there is a finite number of phonon energy states because a phonon cannot have infinite frequency. The frequency of phonon is bound by the medium of its propagation *i.e.* the atomic lattice of the solid. This is not the case in electromagnetic radiation in the Planck's law.

The first normal mode of a transverse phonon and subsequent modes are shown in Fig. 2.25.

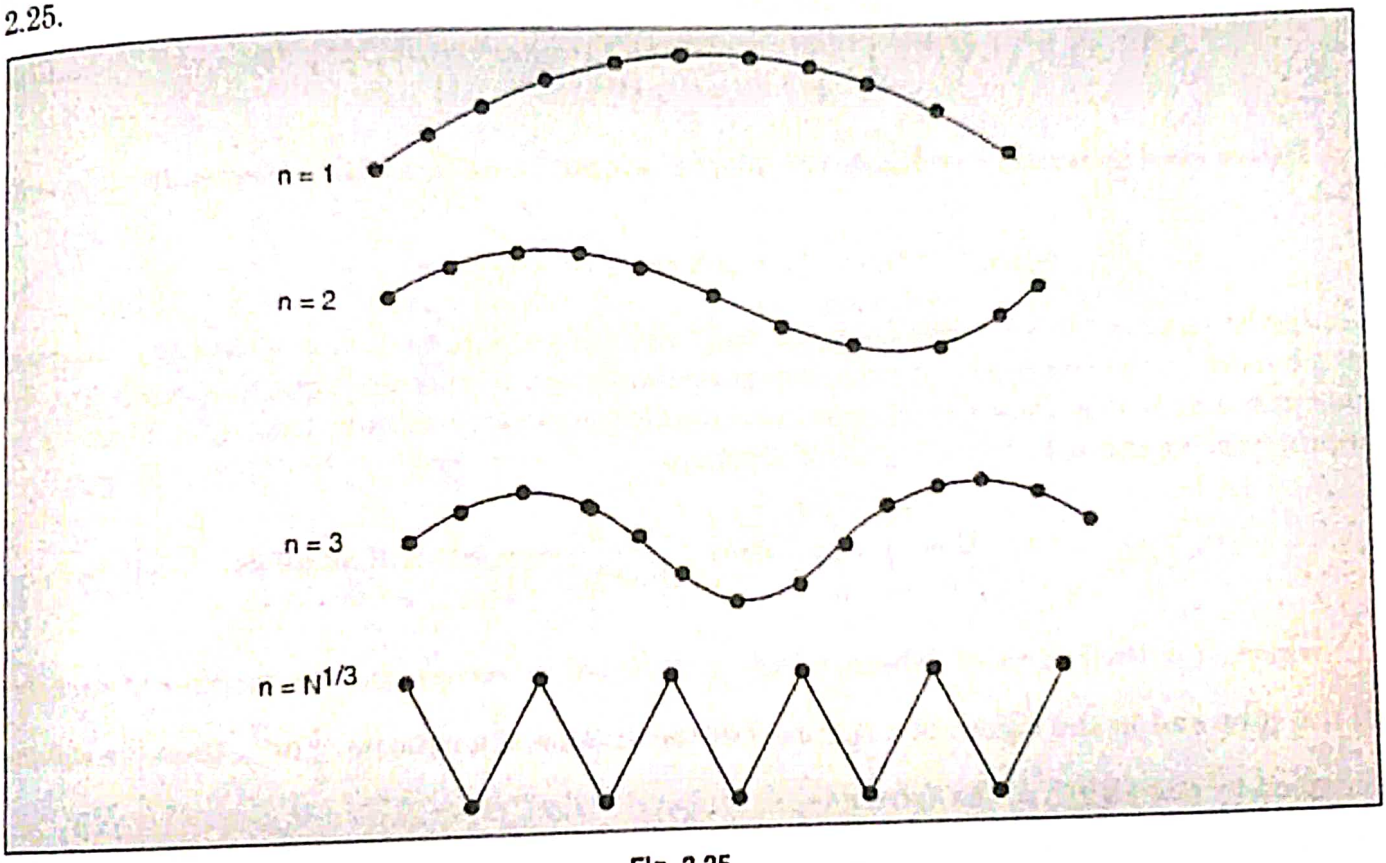


Fig. 2.25.

Debye assumed that the minimum wavelength of a phonon is twice the separation between the atoms. As there are N total number of atoms, so in a cube of side L, there can be $N^{1/3}$ atoms per edge of the cube. The separation of the atoms is given by $L/(N)^{1/3}$ and the expression for the minimum wavelength comes out to be

$$\lambda_{min} = \frac{2L}{(N)^{1/3}}$$

So the upper limit for maximum number of modes is $N^{1/3}$ and the total energy U becomes

$$U = \sum_{n_x}^{N^{1/3}} \sum_{n_y}^{N^{1/3}} \sum_{n_z}^{N^{1/3}} E_n \overline{N}(E_n)$$

when we replace sum in the expression with an integral, the total energy U for slowly varying, well behaved functions becomes

$$U = \int_0^{N^{1/3}} \int_0^{N^{1/3}} \int_0^{N^{1/3}} \left[E(n)\,\overline{N}(E_n)\right] dn_x\, dn_y\, dn_z$$

To calculate $\overline{N}(E_n)$, the number of phonons with energy E_n, we use Bose-Einstein formula of statistical quantum mechanics, as phonons are boson particles, then

$$\overline{N}(E_n) = \frac{1}{e^{E/k_BT} - 1}$$

Substituting the expression for $\overline{N}(E_n)$ in eqn. (*ii*) the energy integral gives

$$U = \int_0^{N^{1/3}} \int_0^{N^{1/3}} \int_0^{N^{1/3}} E(n) \frac{3}{\left(e^{E(n)/k_BT} - 1\right)} dn_x\, dn_y\, dn_z \qquad \text{...(iii)}$$

Debye used spherical coordinates in order to approximate the triple integral given in eqn. (*iii*).

$$(n_x, n_y, n_z) = (n \sin\theta \cos\phi,\ n \sin\theta \sin\phi,\ n \cos\theta)$$

In the case of Planck's law for black body radiations, it is easy to evaluate the integrals for photons as the frequency of electromagnetic radiation is unbound. But this is not true for phonons that is why Debye used spherical coordinates to approximate the triple integrals by approximating the cube by an eighth of a sphere.

$$U \approx \int_0^{\pi/2} \int_0^{\pi/2} \int_0^{R} E(n) \frac{3}{\left(e^{E(n)/k_BT} - 1\right)} n^2 \sin\theta\, dn\, d\theta\, d\phi$$

where R is the radius of sphere, which is obtained by conserving the number of particles in the cube and in the eighth of a sphere. Let the volume of a cube be $\frac{4}{3}\pi r^3$, then the volume occupied by one eighth of the sphere is

$$N = \frac{1}{8}\left(\frac{4}{3}\pi r^3\right)$$

$$r^3 = \frac{24\,N}{4\pi}$$

or

$$r = \left(\frac{6N}{\pi}\right)^{1/3}$$

The total energy U becomes

$$U = \frac{3\pi}{2} \int_0^{R} \frac{h\,v_n\,n}{2L} \frac{n^2}{\left[e^{\frac{h v_n n}{2k_BTL}} - 1\right]} dn$$

Let us put $\frac{h v_n n}{2Lk_BT} = x$ (say)

so that $$U = \frac{3\pi}{2} k_BT \left(\frac{2Lk_BT}{h v_n}\right)^3 \int_0^{\frac{h v_n x}{2k_BLT}} \left(\frac{x^3}{e^x - 1}\right) dx \qquad ...(iv)$$

Let us put the term $\frac{h v_n r}{2Lk_B}$ as T_D where T_D is called Debye temperature. Thus,

$$T_D = \frac{h v_n r}{2Lk_B}$$

$$= \frac{h v_n}{2Lk_B}\left(\frac{6N}{\pi}\right)^{1/3} \qquad \left(\because r = \left(\frac{6N}{\pi}\right)^{1/3}\right)$$

$$= \frac{h v_n}{2Lk_B}\left(\frac{6N}{\pi V}\right)^{1/3}$$

The product of Debye temperature and Boltzman's constant is approximately equal to the phonon energy. **Debye temperature is the temperature at which the highest frequency mode is excited.**

The expression for the specific internal energy is given as

$$\frac{U}{Nk_B} = 9T\left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} \frac{x^3}{e^x - 1} dx$$

$$= 3T\, D_3\left(\frac{T_D}{T}\right) \qquad ...(v)$$

where $D_3(x)$ is the third order Debye function. It is defined as

$$D_n(x) = \frac{n}{x^n} \int_0^x \frac{t^n}{e^t - 1} dt$$

or $$D_3\left(\frac{T_D}{T}\right) = \frac{3}{\left(\frac{T_D}{T}\right)^3} \int_0^{T_D/T} \frac{x^3}{e^x - 1} dx$$

Eqn. (v) can be rewritten as

$$U = 3T\, N k_B\, D_3\left(\frac{T_D}{T}\right)$$

By definition, the specific heat C_V is given by,

$$C_V = \frac{dU}{dT}$$

$$= \frac{d}{dT}\left[3TNk_B\, D_3\left(\frac{T_D}{T}\right)\right]$$

$$= 3\,(Nk_B)\, D_3\left(\frac{T_D}{T}\right)$$

$$= 3\,R\, D_3\left(\frac{T_D}{T}\right)$$

where $N k_B = R$, the universal gas constant.

Special Cases :

(*i*) In lower range of temperature, *i.e.* $T \longrightarrow 0$

$$x = \frac{h\, v_n\, n}{2\,L\, k_B T} \longrightarrow \infty$$

when $T << T_D$, we have $\frac{T_D}{T} \longrightarrow \infty$

Equation (*v*) becomes

$$U = 9\,T\,N\,k_B \left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} \frac{x^3}{e^x - 1}\, dx$$

The solution of the integral $\int_0^{T_D/T} \frac{x^3}{e^x - 1}\, dx = \frac{\pi^4}{15}$, so that

$$U = \frac{9Nk_BT^4}{T_D^3}\left(\frac{\pi^4}{15}\right)$$

Differentiating U with respect to T we get C_V,

$$C_V = \frac{dU}{dT}$$

$$= \frac{d}{dT}\left[\frac{9Nk_BT^4\,\pi^4}{T_D^3 \times 15}\right] = \frac{9Nk_B\pi^4}{15\,T_D^3}\frac{d}{dT}[T^4]$$

$$= \frac{9Nk_B\pi^4}{15\,T_D^3}(4T^3)$$

$$= \left(\frac{12 N k_B \pi^4}{5 T_D^3}\right) T^3$$

i.e. $$C_V \propto T^3$$

This is known as **Debye T^3 law** which is in good agreement with experimental data. A comparison of the results obtained by Einstein's and Debye's theories for specific heat of solid is shown in Fig. 2.26.

It is useful to note that the energy U is directly proportional to T^4, which is similar to result obtained by Stefan's law for the black body radiations. This also confirms that photons and phonons obey the same statistics.

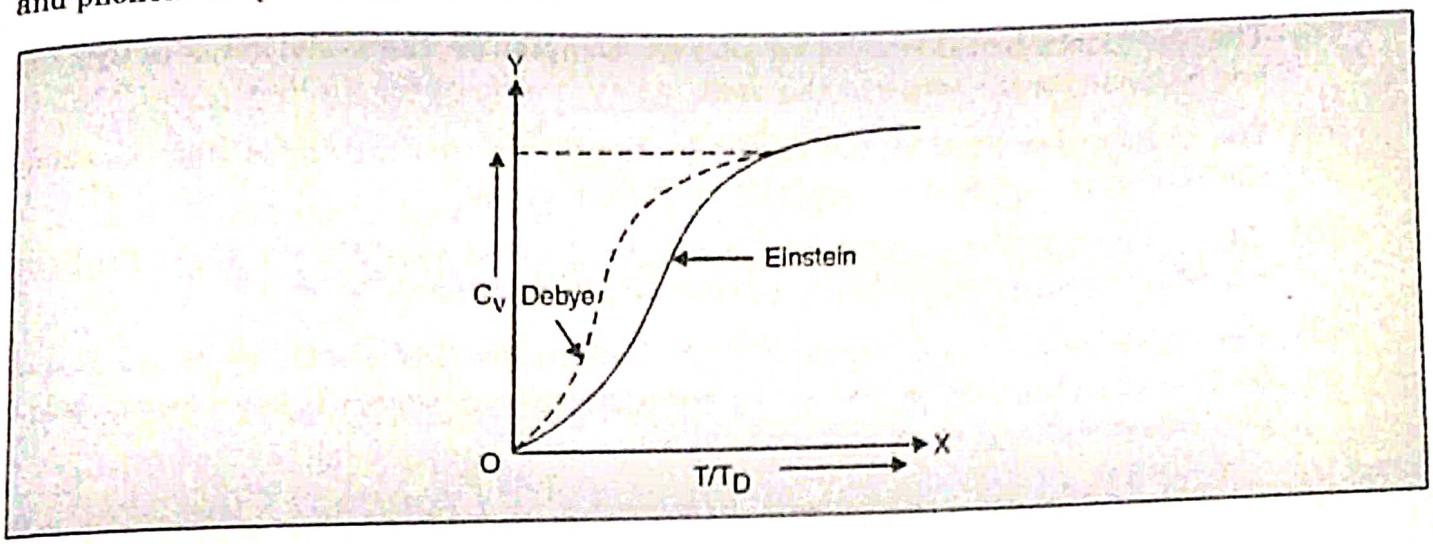


Fig. 2.26.

(ii) At high temperature :

$$T >> T_D$$

hence $$x = \frac{T_D}{T} << 1$$

So that $$e^x - 1 = [(1 + x + ...) - 1]$$

$$= x$$

The eqn. (*v*) of Debye theory can be written as

$$U = 9 N k_B T \left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} \frac{x^3 dx}{x}$$

$$= 9 N k_B T \left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} x^2 dx$$

$$= 9 N k_B T \left(\frac{T}{T_D}\right)^3 \left(\frac{T_D}{T}\right)^3 \left(\frac{1}{3}\right)$$

or $$U = 3\,N\,k_B T$$

or $$U = 3\,R\,T \qquad (\because N k_B = R)$$

Now the specific heat C_V is given as

$$C_V = \left(\frac{dU}{dT}\right)_V = 3R$$

This is Dulong and Petit's law. Thus at very temperatures, Debye theory agrees with both the classical and quantum theory results. This explains that quantum effects are not of much importance at high temperatures.

Limitations of Debye Theory

(i) The continuum model is valid for long wavelengths *i.e.* the model assumes that only low frequencies are active in the solid.

(ii) The assumption that $3N$ modes of vibration is also not justifiable since an elastic continuum is supposed to possess infinite frequencies.

(iii) Since velocities of transverse and longitudinal waves are different, hence the Debye cut off frequency should also be different for these two.

(iv) The experimental results agree with the results from Debye's theory of specific heat fairly well at high temperatures. At low temperatures Debye T^3 law does not hold in the temperature range of less than 0.1 T_D.

(v) According to Debye's theory $T_D = \dfrac{h f_D}{k_B}$ is independent of temperature but actually T_D is found to vary up to 10% with temperature.

(vi) Debye's theory assumes that the solid consists of identical atoms. Hence, the theory is not valid for those crystals, such as NaCl where the atoms are not identical.

(vii) Debye's theory ignores the interatomic interaction and electronic contribution to lattice specific heat.

SOLVED PROBLEMS

PROBLEM 1. If the velocity of sound in air at 10°C is taken to be 340 ms^{-1} and interatomic distance be 6 Å, calculate the value of cut-off frequency assuming a lattice to be linear.

Solution

Velocity of sound $v = 340\ ms^{-1}$

Interatomic distance $a = 5 \times 10^{-10}\ m$

Now we know that

$$v = f\lambda$$

and $$\lambda = 2a,$$

so that we have

$$\vec{v} = f(2a)$$

orfrequency $f = \frac{v}{2a}$

$$= \frac{340}{2 \times 5 \times 10^{-10}} = 34 \times 10^{10} \text{ Hz}$$

PROBLEM 2. **If the velocity of sound in a solid is of the order of 10^3 ms^{-1}, compare the frequency of the sound wave λ = 120 Å for (a) monochromatic system and (b) acoustic waves and optical waves in a diatomic system containing two identical atoms per unit cell of interatomic spacing 1.2 Å.**

Solution

Here, velocity of the sound in solid $v = 10^3\ ms^{-1}$

Wavelength of sound wave $\lambda = 120$ Å $= 120 \times 10^{-10}\ m$

Interatomic spacing $a = 1.2 \times 10^{-10}\ m$

In case of homogeneous line, the frequency,

$$\omega = \frac{2\pi v}{\lambda}$$

$$= \frac{2\pi \times 10^3}{120 \times 10^{-10}} = 0.052 \times 10^{13}$$

$$= 0.52 \times 10^{12} \text{ rad per sec}$$

(*a*) **Acoustic wave** in a diatomic lattice, the frequency varies from

$$\omega = 0 \text{ at } k = 0$$

to $$\omega = \sqrt{\frac{2k}{m}} \text{ where } k = \frac{\pi}{2a}$$

$$\text{velocity } v = a\,\omega = a\sqrt{\frac{2k}{m}}$$

Also $$C_V = \frac{\text{Velocity } v}{\text{interatomic spacing } a}$$

$$= \frac{10^3}{1.2 \times 10^{-10}} = 1$$

$$= 0.83 \times 10^{13} \text{ rad/sec}$$

(*b*) **Optical wave, the frequency varies from**

$$\omega = \sqrt{\frac{4k}{m}} \text{ at } k = U \text{ to } \omega = \sqrt{\frac{2k}{m}} \text{ at } k = \frac{\pi}{2a}$$

At $k = U$, $\omega = \sqrt{2} \times \frac{v}{a}$

or $$\omega = \sqrt{2} \times \frac{10^3}{1.2 \times 10^{-10}} = 1.17 \times 10^{13} \text{ rad/sec}$$

At $$k = \frac{\pi}{2a}, \omega = \frac{v}{a}$$

$$= \frac{10^3}{1.2 \times 10^{-10}} = 0.83 \times 10^{13} \text{ rad/sec}$$

PROBLEM 3. **The unit cell parameter of sodium chloride is 5.22 Å and the modulus of rigidity along [1 0 0] direction is 5.2×10^{10} N m^{-2}. Calculate the wavelength at which an electromagnetic radiation is strongly reflected by the crystal. Atomic mass of sodium and chlorine is 23 and 37 respectively.**

Solution

Here, unit cell parameter $a = 5.22 \times 10^{-10}$ *m*

Modules of rigidity $\eta = 5.2 \times 10^{10}$ *N m*$^{-2}$

The maximum frequency of electromagnetic radiation reflected by sodium chloride crystal is given by

$$\omega_{max} = \sqrt{2k\left(\frac{1}{m_1} + \frac{1}{m_2}\right)}$$

If the extension along [1 0 0] direction has negligible effect on vertical springs, then

$$k = a\eta$$

so that $$\omega_{max} = \sqrt{2\,a\,\eta\left(\frac{1}{m_1} + \frac{1}{m_2}\right)}$$

Now atomic mass of sodium $m_1 = 23$

Atomic mass of chlorine (m_2) = 37

Atomic mass unit= 1.67×10^{-27} *kg*

$$\omega_{max} = \left[\frac{2 \times 5.22 \times 10^{-10} \times 5.22 \times 10^{10}}{1.67 \times 10^{-27}}\left[\frac{1}{37} + \frac{1}{23}\right]\right]^{1/2}$$

$$= \left[\frac{54.288 \times (0.0270 + 0.0434)}{1.67 \times 10^{-27}}\right]^{1/2}$$

$$= \left[\frac{54.288 \times 0.0704}{1.67} \times 10^{+27}\right]^{1/2}$$

$$= [0.2288 \times 10^{26}]^{1/2}$$

$$= \sqrt{0.2288} \times 10^{13}$$

$$= 0.478 \times 10^{13}\ rad\ s^{-1}$$

Wavelength $\lambda = \frac{c}{f}$

$$= \frac{2\pi v}{\omega} = \frac{2\pi \times 10^3}{0.478 \times 10^{13}}$$

$$= 13.13 \times 10^{-10} = 13.13\ \text{Å}$$

PROBLEM 4. **Two sinusoidal waves are superimposed**

$$y_1 = 0.04 \cos (15t - 8x)$$

$$y_2 = 0.06 \cos (9t - 6x)$$

where y_1 and y_2 are in metres and t is in seconds. Calculate the group velocity.

Solution

Here, $y_1 = A \cos (\omega_1 t - k_1 x)$

$y_2 = A \cos (\omega_2 t - k_2 x)$

$\omega_1 = 15$, $\omega_2 = 9$, $k_1 = 8$ and $k_2 = 6$

Now $\Delta\omega = \omega_1 - \omega_2$

and $\Delta k = k_1 - k_2$

Thusgroup velocity $v_g = \frac{\Delta\omega}{\Delta k}$

$$= \frac{(15 - 9)}{(8 - 6)} = 3\ ms^{-1}$$

PROBLEM 5. **Calculate the Einstein's temperature of Cesium if the Einstein's frequency is 1.69×10^{12} Hz.**

Solution

Here, Einstein's frequency $f_E = 1.69 \times 10^{12}\ Hz$

Planck's constant $h = 6.62 \times 10^{-34}\ Js$

Boltzman's constant $k_B = 1.38 \times 10^{-23}$ *SI unit*

Using the relation, $\theta_E = \dfrac{h f_E}{k_B} = \dfrac{6.62 \times 10^{-34} \times 1.69 \times 10^{12}}{1.38 \times 10^{-23}}$

$= 8.1 \times 10 = 81K$

PROBLEM 6. **In the case of vibrations of a monoatomic linear chain, for small ka, the phase velocity is 3880 m s^{-1}. Calculate the group velocity at $k = \left(\dfrac{\pi}{2a}\right)$.**

Solution

Here, phase velocity $v_p = 3880\ ms^{-1}$

$$v_p = \sqrt{\frac{\alpha}{m}}\, a$$

or $$\sqrt{\frac{\alpha}{m}}\, a = 3880 \qquad \ldots(i)$$

Also $\dfrac{ka}{2} = \dfrac{\pi}{4}$, so that

group velocity $v_g = \sqrt{\dfrac{\alpha}{m}}\, a \cos\left(\dfrac{ka}{2}\right)$

$$= \sqrt{\frac{\alpha}{m}}\, a \cos\frac{\pi}{4}$$

$$= \sqrt{\frac{\alpha}{m}}\, \frac{a}{\sqrt{2}} \qquad \ldots(ii)$$

Divide eqn. (*ii*) by eqn. (*i*), we get

$$\frac{v_g}{v_p} = \frac{1}{\sqrt{2}}$$

or $$v_g = \frac{v_p}{\sqrt{2}} = \frac{3880}{\sqrt{2}} = 2743.9\ \text{ms}^{-1}$$

PROBLEM 7. **For a metal, Young's modulus is 1.2×10^{11} N m^{-2} and interatomic spacing a 1.46 Å. The mass of its atom is 5.464×10^{-25} kg. Determine the force constant α and the characteristic vibrational frequency f of the atoms.**

Solution

Here, $\alpha = Ya$

$= 1.2 \times 10^{11} = 1.46 \times 10^{-10}$

$= 1.752 \times 10\ N\ m^{-1}$

Now vibrational frequency f is given by

$$f = \frac{\omega}{2\pi} = \frac{1}{2\pi}\sqrt{\frac{\alpha}{m}}$$

$$= \frac{1}{2 \times 3.14}\sqrt{\frac{1.752 \times 10}{5.464 \times 10^{-25}}}$$

$$= \frac{1}{6.28}\sqrt{0.320 \times 10^{26}}$$

$$= \sqrt{\frac{0.320}{6.28}} \times 10^{13} = 0.566 \times 10^{13} \text{ Hz}$$

PROBLEM 8. **How many longitudinal modes are there for (a) linear monoatomic lattice and (b) a linear diatomic lattice of interatomic spacing of 1 Å and of length 0.01 m ?**

Solution

Since length L = 0.01 m

and interatomic spacing $a = 10^{-10}$ m

Hence the number of atoms $N = 10^{10}$

Number of modes for monoatomic fixed lattice = 10^{10}

Number of modes for periodic monoatomic lattice = $\frac{N}{2} = \frac{10^{10}}{2} = 0.5 \times 10^{10}$

Number of modes for fixed diatomic lattice = $\frac{N}{2} = 0.5 \times 10^{10}$

Number of modes for periodic diatomic lattice = $\frac{N}{4} = 0.25 \times 10^{10}$

PROBLEM 9. **The Debye temperatures of two isomorphous ionic solids are 246 K and 188 K respectively. If the lattice heat capacity of the first ionic solid at 10K is 0.0263 J mole^{-1} K^{-1}, calculate the heat capacity of the second ionic solid at the same temperature.**

Solution

Here, $(C_V)_2 = 0.0263\ J\ mole^{-1}\ K^{-1}$

Debye temperature $(T_D)_1 = 246\ K$

Debye temperature $(T_D)_2 = 188\ K$

Now, we know that at low temperature,

$$C_V \propto \left(\frac{T}{T_D}\right)^3$$

So, at same temperature

$$\frac{(C_V)_2}{(C_V)_1} = \left[\frac{(T_D)_1}{(T_D)_2}\right]^3$$

or $$(C_V)_2 = (C_V)_1 \left[\frac{(T_D)_1}{(T_D)_2}\right]^3$$

$$= 0.0263 \left[\frac{246}{188}\right]^3$$

$$= 0.0263 \times (1.308)^3$$

$$= 0.0263 \times 2.2378$$

$$= 0.0588 \text{ J mole}^{-1}\text{K}^{-1}$$

PROBLEM 10. At very low temperature, the specific heat of material varies with temperature as per Debye T^3 law. If the Debye temperature is 425 K then find the quantity of heat required to raise the temperature of 4 moles of material through 27°C to 40°C.

Solution

Here, no. of moles = 4

Debye temperature $T_D = 425\ K$

Temperature $T_1 = 27°C$

$= 27 + 273 = 300\ K$

Temperature $T_2 = 40 + 273 = 313\ K$

Gas constant $R = 8.31\ J\,K^{-1}\ mole^{-1}$

At low temperature, according to Debye's theory the specific heat is given by

$$C_V = \frac{12}{5}\pi^4 R\left(\frac{T}{T_D}\right)^3$$

Now, the quantity of heat required to raise the temperature of 4 mole of solid through small temperature from T_1 to T_2 is

$$dQ = n\ C_V\, dT$$

$$= n\,\frac{12}{5}\pi^2 R\left(\frac{T}{T_D}\right)^3 dT$$

The total quantity of heat can be obtained by integrating *w.r.t.* T.

$$Q = \int_{300\ K}^{313\ K} n \times \frac{12}{5} \times \pi^2 \times R \times \left(\frac{T}{T_D}\right)^3 dT$$

$$= 4 \times \frac{12}{5} \times \frac{(3.14)^2 \times (8.31)}{(425)^3} \times \frac{1}{4}[(313)^4 - (300)^4]$$

$$= 0.00000256\ [9597924961 - 8100000000]$$

$$= 0.00000256 \times 9597924961$$

$$= 3834.6\ J\ mole^{-1}\ K^{-1}$$

PROBLEM 11. Calculate the specific heat for aluminium at 0°C and Debye temperature of 370 K.

Solution

Here, Debye temperature $T_D = 370\ K$

Avogadro's number $N = 6.023 \times 10^{23}\ mole^{-1}$

Boltzman's constant $k_B = 1.38 \times 10^{-23}\ J\ K^{-1}$

Temperature $T = 0°C$

$$= 0 + 273 = 273\ K$$

We know that the specific heat C_V is given by

$$C_V = \frac{12}{5}\pi^4 N k_B \left(\frac{T}{T_D}\right)^3 \text{ if } T << T_D$$

$$= \frac{12}{5} \times (3.14)^4 \times 6.023 \times 10^{23} \times 1.38 \times 10^{-23} \times \left(\frac{273}{370}\right)^3$$

$$= 2445.37\ \text{J mole}^{-1}\ \text{K}^{-1}$$

CONCEPTUAL QUESTIONS

Q. 1. What are lattice vibrations ?

Ans. Lattice vibrations are the vibrations of the atoms about their mean position in the solid. These vibrations cause thermal properties such as heat capacity, thermal conductivity, thermal expansion etc. of the solids.

Q. 2. How do you consider the concept of the atoms in the lattice dynamics ?

Ans. In lattice dynamics, the atoms are considered as point masses averaged in some effective potential, defined by their mutual interactions which determine their motion.

Q. 3. What is a phonon ?

Ans. Phonon is a quantum mechanical description of an elementary vibrational motion in which a lattice of atoms or molecules uniformly oscillates at a single frequency. In other words, phonon is the quanta of energy in elastic wave.

Q. 4. Do phonons have a mass ?

Ans. No, phonons are massless boson particles resulting from the violation of the continuous translational symmetry of free space, by the crystal lattice. Although phonons are massless but they do have momentum by virtue of their wavelength.

Q. 5. What is optional phonon ?

Ans. Optical phonon results from out of phase vibrations between neighbouring atoms within the unit cell.

Q. 6. Which statistics does phonon obey ?

Ans. Phonon obeys Bose-Einstein's statistics. This is because phonons are indistinguishable and these particles do not obey Pauli's exclusion principle.

Q. 7. What is the cut off frequency for a linear monoatomic lattice if the atomic spacing (a) is 1 Å and velocity of sound is 330 ms^{-1} at 0°C.

Ans. The cut off frequency $f = \dfrac{\text{velocity}}{a/2}$

$$= \frac{2v}{a} = \frac{2 \times 340}{10^{-10}} = 680 \times 10^{10}\ Hz$$

Q. 8. What properties are exhibited by the solids due to the execution of coupled vibrations by the atoms of the crystal.

Ans. A solid crystal oscillates in normal mode due to

(*i*) its internal energy

and (*ii*) the effect of some external forces which may be mechanical or electromagnetic.

The vibrations of the first type exhibit the properties related to thermal properties whereas the vibrations of the latter type are associated with acoustic and some optical properties of solids.

Q. 9. Do phonon possess momentum ? How a phonon is related to momentum?

Ans. A phonon on a lattice really has no momentum in the physical sense. On the other hand, a phonon of wavelength $\vec{k}$ interacts with particles such as photon, electron and neutron as if it possesses a momentum $\hbar\vec{k}$ in the same way as photon of equivalent wavelength λ. The momentum $\hbar\vec{k}$ is known as crystal momentum.

Q. 10. Mention those properties which are common in both photons and phonons ?

Ans. (*i*) A phonon and a photon both show the wave particle duality.

(*ii*) The momentum of a photon $\vec{p} = \dfrac{h}{\lambda} = \hbar k$ where k is the propagation constant is similar to crystal momentum in the case of a phonon.

(*iii*) The energy of a photon of frequency f is $h f$. This is true for a phonon also.

(*iv*) Phonon and a photon both are indistinguishable particles and follow Bose-Einstein's statistics.

Q. 11. What is the difference between a phonon and a photon ?

Ans. (*i*) A photon is a quantum of energy in electromagnetic waves whereas a phonon is a quantum of energy in an elastic wave.

(*ii*) A photon travels with the velocity of light whereas the phonon moves with the velocity of sound in the solids.

(*iii*) Photon does not require any material medium for its propagation whereas a phonon requires a material medium to travel.

(*iv*) A phonon is emitted or absorbed in the inelastic scattering of a photon by a crystal. The reverse process *i.e.* emission or absorption of a photon by scattering of a phonon is not possible.

Q. 12. For what values of frequencies, a monoatomic one dimensional lattice behaves as a dispersive medium ?

Ans. In monoatomic lattice, the dispersion effects are negligible at low frequency ($k \to 0$) and lattice behaves as a continuous for frequencies less than $\sqrt{\frac{4f}{m_2}}$, the lattice behaves as dispersive medium. It acts as a low pass filter and can propagate a number of wavelengths at the same frequencies. For frequency $\omega = \sqrt{\frac{4f}{m_2}}$, the standing waves are formed and there is no transfer of signal or energy through the lattice.

Q. 13. Describe the nature of motion in the case of monoatomic linear lattice when group velocity is equal to zero.

Ans. At $v_g = 0$, $k = \frac{\pi}{a}$ or $\lambda \longrightarrow 2a$, the phase of neighbouring atoms differs by π and the nature of motion is simply a standing wave. The situation is similar to Bragg's first order reflection in *X*-ray diffraction for normal incidence.

Q. 14. Can we count number of phonons at fixed frequency ?

Ans. The number of phonon is not a fixed value. If one atom begins to vibrate, then few phonons are created. When the vibrations stop, the phonons disappear. Although we cannot determine the number of phonons, at a fixed temperature, we know the probability of having n phonons.

Q. 15. Prove that, for a one dimensional monoatomic lattice, dispersion curve meets the zone boundary in a normal direction.

Ans. The dispersion curve is given by the expression

$$\omega = 2\sqrt{\frac{\alpha}{m}} \sin\left(\frac{ka}{2}\right)$$

$\therefore$ the group velocity $v_g = \dfrac{d\omega}{dk}$

$$= 2\sqrt{\frac{\alpha}{m}}\left(\frac{a}{2}\right)\cos\left(\frac{ka}{2}\right)$$

Zone boundary is defined by

$$k = \pm\frac{\pi}{a}, \text{ for which}$$

$$\cos\frac{ka}{2} = \cos\left(\pm\frac{\pi}{2}\right) = 0$$

Hence the group velocity $\dfrac{d\omega}{dk}$ is equal to zero at zone boundary *i.e.* the dispersion curve is perpendicular to the zone boundary.

Q. 16. Prove that the group velocity at the zone boundary of the optic branch as well as the acoustic branch of lattice vibrations of a diatomic linear chain is zero.

Ans. The relevant dispersion relation is

$$\omega_{\pm}^2 = \alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm \left[\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4\sin^2 ka}{m_1 m_2}\right]^{1/2}$$

where + ve sign denotes optic branch and – ve sign denotes the acoustic branch

$$\frac{d\omega_{\pm}^2}{dk} = \pm\frac{1}{2}\left[\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4\sin^2 ka}{m_1 m_2}\right]$$

$$\times\left[-\frac{4a}{m_1 m_2}\right] 2\sin ka\cos ka$$

$$\frac{d\omega_{\pm}^2}{dk} = \mp\left(\frac{2a}{m_1 m_2}\right)\left[\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4\sin^2 ka}{m_1 m_2}\right]^{-1/2} \sin 2ka$$

At zone boundary, $k = \pm\dfrac{\pi}{2a}$, we have,

$$\sin 2ka = \sin(\pm\pi) = 0$$

or $$\frac{d}{dk}(\omega_{\pm}^2) = 0$$

Hence, group velocity $v_g = \dfrac{d\omega_{\pm}}{dk} = 0$

Q. 17. Which one is the most reliable model for phonons ?

Ans. Einstein's model is reliable and adequate for interpreting the optical branch while Debye model is successful in explaining the acoustical branch of the dispersion curve.

Q. 18. Why one dimensional chain in lattice dynamics behaves as a low pass filter ?

Ans. The maximum frequency that can be propagated through one dimensional chain is

$$\omega_0 = \frac{\pi v}{a}$$

where v is the velocity of sound in crystal which is of the order of $10^4\ ms^{-1}$ and a is the interatomic separation distance of the order of 1 Å. Therefore, ω_0 is approximately 10^{14} rad s^{-1}, so one dimensional chain allows only low frequencies to pass. That is why one dimensional chain behaves as a low pass filter.

Q. 19. What is the difference between phonon and ordinary oscillatory motion of atoms in metals ?

Ans. Phonons are quantised form of oscillatory motion. Therefore they need energy packet to excite them. Ordinary oscillatory motion of atoms is a bounded motion because the displacement in oscillatory motion on either side of the mean position has a fixed value.

Q. 20. Do phonons transmit heat ?

Ans. With the increase of temperature, more phonons are created. In terms of Planck's distribution law, we have

$$< n > = \frac{1}{e^{\hbar\omega/k_B T} - 1}$$

where $< n >$ is the expectation value of the number of phonons of a given frequency which exist at a given temperature T and k_B is Boltzman's constant which converts temperature into units of energy. Planck's distribution law is used to determine the specific heat at constant volume C_V which describes how much the temperature is required to heat a material when it absorbs some energy.

Q. 21. Why cannot optical phonons contribute to heat transfer ?

Ans. Because optical phonons have a small group velocity. These phonons do not transport thermal energy through a solid quickly enough to have a significant effect on thermal transport.

Q. 22. Write the temperature dependence of lattice heat capacity at low temperatures.

Ans. At very low temperatures close to zero kelvin, the heat capacity decreases sharply and follows T^3 law for insulators and T-law for metals.

According to Dulong and Petit's law the specific heat of all solids is constant and independent of temperature.

According to Einstein's theory, the specific heat at low temperature $T << \theta_E$ where θ_E is the Einstein's temperature, the heat capacity of lattice is proportional to $e^{-\theta_E/k_B T}$.

According to Debye's theory at low temperatures the specific heat is proportional to T^3 which is known as Debye T^3 law.

Q. 23. What is the physical significance of Debye temperature ?

Ans. The significance of Debye temperature is that at temperature $T >> T_D$ where T_D is Debye temperature, the specific heat at constant volume C_V has the same value as given by Dulong-Petit's law or Einstein's theory.

At very low temperatures $T << T_D$ the specific heat at constant volume obeys T^3 law.

Q. 24. How did Debye modify the Einstein's model of specific heat ?

Ans. Debye suggested that the atoms in the crystal are coupled together and so these coupled atoms oscillate with frequencies whose values vary over a wide range. He also opined that all the possible mode of vibrations are limited by number of atoms in the crystal which produce frequency spectrum.

Q. 25. What is the basic difference between Einstein's theory and Debye theory?

Ans. The basic difference between the two theories is that Debye considers the vibrational modes of a crystal as a whole whereas Einstein's considered the vibrations of single atom assuming the atomic vibrations to be independent of each other.

CHAPTER AT A GLANCE

1. **Lattice Vibration** is the study of vibrations of the atoms about their mean position in a solid. These vibrations are almost responsible for the thermal properties, heat capacity, thermal conductivity, thermal expansion of solids and contribute the greater part of the heat capacity of metals.
2. **Acoustical and optical properties** of solids are caused when a solid body oscillates freely in its normal modes and under the influence of dynamic external forces such as mechanical or electromagnetic force.
3. **The Dispersion relation** for one dimensional monoatomic lattice with nearest neighbour interaction is $\omega = \omega_0 \sin \frac{ka}{2}$ where $\omega_0 = \sqrt{4\alpha/m}$ is the cut off frequency and α is interatomic force constant.
4. **Phonon** is the quanta of energy of lattice vibration. Most of the concepts which apply to photons also apply to phonons like wave particle duality, momentum $\hbar k$ and energy $(\hbar\omega)$ etc.
5. **A normal mole** is a correlated motion of the atoms that has a characteristic wave vector and frequency. If this motion gets started, it will continue to move for ever neglecting the an harmonic terms such as friction.
6. In the **long wavelength limit,** a solid is treated as a continuous medium because the wavelength is much greater than the lattice constant.
7. The **linearity** of the dispersion curve is near $k = 0$ in the long wavelength limit and the curve saturates at large value of k.
8. **Low pass filter** is the term for the lattice as only the waves whose frequencies are lower than ω_0 are transmitted and modes with frequencies eceeding ω_0 are heavily attenuated.

9. **Wave Vector Selection Rules** which governs the process of creation of phonon of wavelength $\vec{K}_{final}$ by inelastic scattering of a photon or neutron from wavevector $\vec{K}$ and $\vec{K}'$ is

$$\vec{K} = \vec{K}' + \vec{K}_{final} + \vec{G}$$

where $\vec{G}$ is a reciprocal lattice vector.

10. **Dulong and Petit's law** states that the specific heat of a solid is constant and is equal to $3R$. The specific heat is independent of temperature. The law is valid only for high temperatures, at low temperatures the specific heat decreases and ultimately becomes zero at zero kelvin.

11. **Einstein's theory** removes the discrepancy in the Dulong and Petit's law by treating the vibration of atom in a crystal quantum mechanically.

12. The **average thermal energy** in Einstein's theory for the vibrations of atoms is given by

$$\overline{U} = \frac{\hbar\omega}{e^{\hbar\omega/k_BT} - 1}$$

where $\hbar = \frac{h}{2\pi}$ and $\omega = 2\pi f$. This energy approaches the classical result k_BT only at high temperatures.

13. The **specific heat** in Einstein's theory by treating the atoms as independent oscillators is given by

$$C_V = 3Nk_B\left(\frac{\theta_E}{T}\right)^2 \frac{e^{\theta_E/T}}{\left[e^{\theta_E/T} - 1\right]^2}$$

14. **Debye's theory** treats the atoms not as independent oscillators but as coupled oscillators vibrating collectively as sound waves.

15. **Debye T^3 law** is in agreement with observations. The expression for the specific heat C_V in Debye's theory approaches the classical value $3R$ at high temperatures but at low temperatures C_V tends to approach T^3.

MULTIPLE CHOICE QUESTIONS

For each question given below choose a correct option.

1. **In case of monoatomic one dimensional lattice the range of $\vec{K}$ values for first Brillouin zone is**

(a) $0 \le \vec{K} \le \frac{\pi}{a}$ (b) $0 \le \vec{K} \le \frac{2\pi}{a}$

(c) $\frac{-\pi}{a} \le \vec{K} \le \frac{\pi}{a}$ (d) $\frac{-\pi}{2a} \le \vec{K} \le \frac{\pi}{2a}$

2. **A phonon is emitted or absorbed in**
   (a) Elastic scattering of a photon by a crystal
   (b) Inelastic scattering of a photon by a crystal
   (c) Both the elastic and inelastic scattering of a photon by a crystal
   (d) none of the above.

3. **A phonon is**
   (a) a photon
   (b) a quanta of energy of lattice vibration
   (c) cation
   (d) anion

4. **In case of elastic vibrations in continuous medium if v_g and v_p represent the group velocity and phase velocity respectively then**
   (a) $v_g = v_p$
   (b) $v_g < v_p$
   (c) $v_g > v_p$
   (d) none of the above

5. **The knowledge of lattice vibrations is useful for providing information about**
   (a) specific heat
   (b) thermal conductivity
   (c) thermal expansion
   (d) all the above

6. **Einstein's theory of lattice vibration is based on the quantum theory of**
   (a) Schrodinger
   (b) Dirac
   (c) Planck
   (d) Heisenberg

7. **For a linear diatomic chain, the long wavelength satisfies the condition**
   (a) $k \to 0$
   (b) phase velocity $\longrightarrow \infty$
   (c) group velocity $\longrightarrow 0$
   (d) all the above

8. **In acoustic branch**
   (a) two consecutive atoms displace in same direction
   (b) two consecutive atoms displace in opposite direction
   (c) all the particles are at rest
   (d) none of the above

9. **As the temperature approaches zero the lattice contribution to heat capacity of solid approaches to**
   (a) infinity
   (b) zero
   (c) one
   (d) any value between zero and infinity

10. **Debye theory of heat capacity considers the vibrations of the crystal is:**
    (a) the vibrational motion of the atoms located at lattice points
    (b) independent and equal
    (c) a giant molecule which is incompressible and inelastic medium
    (d) in number of modes with crystal as a continuous media

11. **A crystal lattice behaves like an elastic continuums for the propagation of waves. It refers to :**
    (a) Debye's theory of specific heat
    (b) Dulong and Petit's law
    (c) Einstein's theory of specific heat
    (d) none of above

12. **A dispersion relation links angular frequency ω with :**
    (a) wavelength
    (b) velocity
    (c) refractive index
    (d) wave number

13. **In case of diatomic lattice at the zone boundary we have in acoustic branch :**
    (a) both heavy as well as light particles are at rest
    (b) both heavy as well as light particles are in motion
    (c) only light particles are at rest
    (d) only heavy particles are at rest

14. **When light mass $m_1 \longrightarrow 0$, optical branch disappears having the dispersion relation of a monoatomic lattice as follows :**

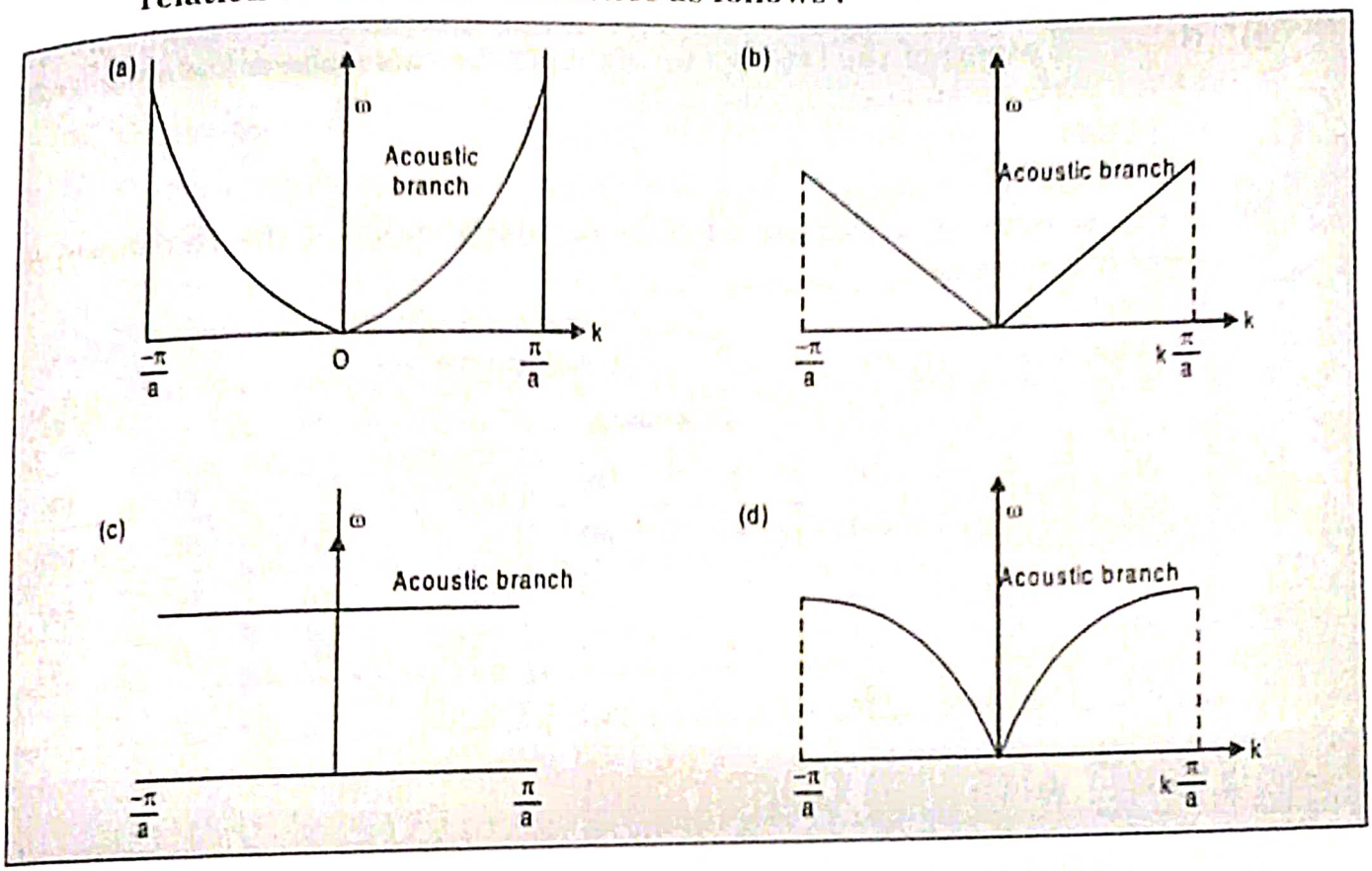


Fig. 2.27

15. **In the harmonic model of lattice vibrations :**
    (a) there is no thermal expansion
    (b) there is a thermal expansion
    (c) the heat capacity is not constant at higher temperature
    (d) isothermal and elastic constants are different

16. **In the Debye model for a three dimensional crystal the internal energy U at low temperature is given by**
    (a) $U \propto T$ (b) $U \propto T^2$
    (c) $U \propto T^3$ (d) $U \propto T^4$

17. **Debye constant could be derived from**
    (a) specific heat (b) elastic data
    (c) both the above (d) none of the above

18. **Phonons are quantised form of ..... motion :**
    (a) linear (b) rotatory
    (c) oscillatory (d) none of the above

19. **To calculate the kinetic energy of a travelling neutron by measuring the time taken between the two fixed points where the distance is known, we use the method :**
(a) Parabolic method (b) Time of high method
(c) Time measurement method (d) Phono spectrum method

20. **The particles responsible for the interactions of a solid with light because they have higher frequencies are called :**
(a) photon (b) phonon
(c) acoustical phonon (d) optical phonon

21. **When the atoms of the lattice vibrate with the same phase and amplitudes about their mean position, the particles are said to be**
(a) photon (b) phonon
(c) acoustical phonon (d) optical phonon

22. **If the velocity of a moving wave is not dependent on the frequency, the solid is known as :**
(a) crystalline (b) non-crystalline
(c) dispersive (d) non-dispersive

Answers

1.	(c)	2.	(b)	3.	(b)	4.	(a)	5.	(a)
6.	(c)	7.	(d)	8.	(a)	9.	(b)	10.	(d)
11.	(a)	12.	(d)	13.	(c)	14.	(d)	15.	(a)
16.	(d)	17.	(c)	18.	(c)	19.	(b)	20.	(d)
21.	(c)	22.	(d)						

SHORT ANSWER QUESTIONS

1. Define a photon.
2. Which crystals exhibit optical phonon modes ?
3. Which restriction on the k-values for the lattice vibrations are found for one dimensional chain with one and two atoms per cell respectively ?
4. Is the group velocity same for optical and acoustical lattice vibration ? Explain.
5. What is common between phonon and a photon ?
6. How does elastic vibrations differ from electromagnetic waves ?
7. Which statistics does phonon obey ?
8. At what temperatures the result of Dulong-Petit's law is in agreement with the experimental values ?
9. Plot a graph to show the general temperature dependence of specific heats of solids?
10. Give the expression for the average energy for one dimensional oscillator according to classical theory of specific heats ?

11. When does the expression for specific heat of solid in Debye's theory approach the classical value $3R$?

12. State Debye T^3 law.

LONG ANSWER QUESTIONS

1. Discuss the quantization of lattice vibrations ? Explain the concepts of phonon ? Do they really exist ?

2. Describe the lattice vibrations of monoatomic linear lattice and obtain an expression for the dispersion relation for lattice vibrations of monoatomic linear chain ?

3. Obtain the various vibrational modes of a linear monoatomic lattice.

4. Derive an expression for the energy and momentum of phonons and explain normal process and umklap process ?

5. Obtain an expression using the inelastic scattering of photons by phonons, for the frequency of phonon emitted in the process.

6. What is a phonon ? Describe the vibrational modes of a diatomic linear lattice ? Name the different branches of the dispersion relation curve ? What is the difference between the two branches?

7. Define molar specific heat at constant volume and lattice heat capacity ? Explain Dulong and Petit's law. What are the limitations of this law?

8. What are the assumptions of Einstein's theory of specific heat of solids ? Derive an expression for lattice heat capacity following Einstein's theory ? Discuss the relation at very high and at very low temperatures. Give the predictions of this theory and compare with the experimental observations.

9. Write the basic drawbacks of Einstein's theory of specific heats ? Using the assumptions derive an expression for the lattice specific heat according to Debye theory.

10. Explain in detail the high and low temperature limits and define Debye – T^3 law. Give limitations of Debye model and compare it with that of Einstein's theory.

11. What is Debye frequency and Debye temperature? Give their physical significance.

UNSOLVED NUMERICAL PROBLEMS

1. If the velocity of sound in a solid is taken to be $3 \times 10^3\ ms^{-1}$ and interatomic distance as $5 \times 10^{-10}\ m$, calculate the cut off frequency assuming the lattice to be linear. [Ans. $3 \times 10^{12}\ Hz$]

2. If the velocity of sound in a solid is of the order of $10^3\ ms^{-1}$, compare the frequency of the sound wave $\lambda = 20$ Å for (*a*) monochromatic system and (*b*) acoustic waves and optical waves in a diatomic system containing two identical atoms per unit cell of interatomic spacing 2.2 Å. [Ans. $\omega = 3.14 \times 10^{12}$ rad/sec, 4.54×10^{12} rad/sec 6.42×10^{12} rad/sec and 4.54×10^{12} rad/sec]

3. Calculate the wavelength at which an electromagnetic radiation is entirely reflected by sodium chloride crystal having unit cell parameter as 5.65 Å. The modulus of rigidity along [1 0 0] direction is $6 \times 10^{10}\ N\ m^{-2}$ and the atomic weights of Na and Cl are 23 and 37 respectively. [Ans. $3.67 \times 10^{-5}\ m$]

4. If two simple harmonic travelling plane waves

$$y_1 = 0.03 \sin (7t - 10x)$$

$$y_2 = 0.03 \sin (5t - 8x)$$

are superposed. Calculate the velocity of the resulting wave group. [Ans. $1\ ms^{-1}$]

5. Calculate the Einstein's temperature of a metallic solid if the Einstein's frequency is $10^{12}\ Hz$. [Ans. $48\ K$]

6. In the case of vibrations of a monoatomic linear chain, for small ka, the phase velocity is $5000\ ms^{-1}$. Calculate the group velocity at $k = \frac{\pi}{2a}$. [Ans. $3536\ ms^{-1}$]

7. For a metal, Young's modulus is $Y = 2 \times 10^{11}\ N\ m^{-2}$ and interatomic spacing $a = 2.8$ Å. The mass of its atom is $10.556 \times 10^{-26}\ kg$. Calculate the value of force constant a and the characteristic vibrational frequency of the atoms.

[Ans. $56\ N\ m^{-1}$, $3.66 \times 10^{12}\ Hz$]

8. The Debye temperature of two isomorphous ionic solids are 281 K and 230 K respectively. If the lattice heat capacity of the first ionic solid at 5 K is 0.016 $J\ mole^{-1}\ K^{-1}$, then estimate the heat capacity of the second solid at 5 K.

[Ans. $0.0291\ J\ mole^{-1}\ K^{-1}$]

9. A very low temperature, the specific heat of rock salt varies with temperature according to Debye T^3 law. If the Debye temperature is 375 K, then find the quantity of heat required to raise the temperature of 2 moles of salt through 15° to 40° C. [Ans. 44.54 Cal]

10. Calculate the specific heat for aluminium at 300 K and its Debye temperature 375 K. [Ans. $995\ kJ/k\ mole\ K$]

□□□

Syllabus

ALL INDIAN UNIVERSITIES & AUTONOMOUS COLLEGES, ODISHA

Physics- XII: Solid State Physics

(Credits; Theory-04) *Theory : 40 Classes (1 hr duration)*

UNIT – I

Crystal Structure: Solids : Amorphous and Crystalline Materials. Lattice Translation Vectors. Lattice with a Basis – Central and Non-Central Elements. Unit Cell. Miller Indices. Types of Lattices, Reciprocal Lattice. Brillouin Zones. Diffraction of X-rays by Crystals. Bragg's Law. Atomic and Geometrical Factor.

Elementary Lattice Dynamics: Lattice Vibrations and Phonons: Linear Monoatomic and Diatomic Chains. Acoustical and Optical Phonons. Qualitative Description of the Phonon Spectrum in Solids. Dulong and Petit's Law, Einstein and Debye theories of specific heat of solids. T^3 law

UNIT – II

Magnetic Properties of Matter: Dia-, Para-, Ferri- and Ferromagnetic Materials. Classical Langevin Theory of dia-and Paramagnetic Domains. Curie's law, Weiss's Theory of Ferromagnetism and Ferromagnetic Domains. Discussion of B-H Curve. Hysteresis and Energy Loss.

Dielectric Properties of Materials: Polarization. Local Electric Field at an Atom. Depolarization Field. Electric Susceptibility. Polarizability. Clausius Mosotti Equation. Classical Theory of Electric Polarizability.

Lasers: Einstein's A and B coefficients. Metastable states. Spontaneous and Stimulated emissions. Optical Pumping and Population Inversion. Three–Level and Four-Level Lasers. Ruby Laser and He-Ne Laser.

UNIT – III

Elementary band theory: Kronig Penny model Band Gap. Conductor, Semiconductor (P and N type) and insulator. Conductivity of Semiconductor, mobility, Hall Effect. Measurement of conductivity (04 probe method) & Hall coefficient.

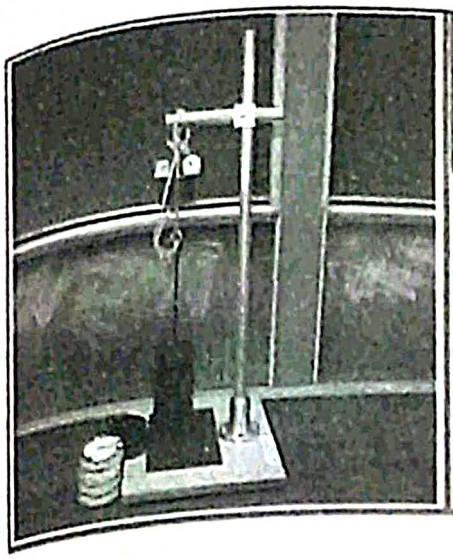
Superconductivity: Experimental Results. Critical Temperature, Critical magnetic field. Meissner effect. Type I and type II Superconductors, London's Equation and Penetration Depth. Isotope effect. Idea of BCS theory (No derivation)

UNIT – II

3. *MAGNETIC PROPERTIES OF MATTER*

4. *DIELECTRIC PROPERTIES OF MATERIALS*

5. *LASERS*



Chapter 3

MAGNETIC PROPERTIES OF MATTER

INTRODUCTION

The magnetic properties of solids originates from motion of electrons. Every substance consists of atoms and electrons in each atom are revolving around the nucleus in various orbits. An electron revolving in an orbit around the nucleus is equivalent to circular electric current and behaves like a magnet and possesses a magnetic moment. Since most of atoms include several electronic orbits, their orbital magnetic moments are not usually parallel to each other and sense of rotation is not essentially the same. Hence in case the arrangements of orbits is such that the vector sum of magnetic moments is not zero, then atom has a resultant magnetic moment. Such substances possess a permanent magnetic moment and are called paramagnetic substances. When such substances are placed in an external magnetic field, their atoms will rotate in the field direction increasing the magnetic induction.

If the arrangements of orbits is such that the vector sum of magnetic moments is zero. Such atoms has zero resultant moment. When such an atom is placed in an external magnetic field, there is no directive rotating action on the atom, although the field cause a rotating action due to its influence on individual electronic orbits. This action produces an induced magnetic moment. This induced magnetic moment will be in direction opposite to the applied field according to Lenz's law and hence tends to decrease the magnetic induction. Substances consists of such atoms or molecules are called diamagnetic substances.

3.1 SOME IMPORTANT TERMS

The following terms and concepts are used in the field of magnetism.

1. Magnetic Intensity

Consider a magnetic field B_0 exists inside vacuum, then magnetic intensity is given by relation

$$H = \frac{B_0}{\mu_0} \qquad \ldots(3.1)$$

where $\mu_0 = 4\pi \times 10^{-7}$ tesla metre ampere^{-1} (i.e. TmA^{-1}) is absolute permeability of vacuum.

The unit of magnetic intensity is

$$H = \frac{\text{Tesla}}{\text{Tesla metre amp}^{-1}} = \frac{1}{\text{Metre ampere}^{-1}} = \text{ampere metre}^{-1} \text{ or } Am^{-1}$$

Magnetic intensity is also known as **magnetic field strength.** The unit Am^{-1} is also equivalent to $Nm^{-2}T^{-1}$ or NWb^{-1}.

2. Intensity of Magnetization

It is defined as the magnetic moment developed per unit volume, when a magnetic material specimen is subjected to magnetizing field.

It is denoted by (I)

If magnetic dipole moment M is acquired by a specimen of volume V due to the magnetizing field, then intensity of magnetization is given as

$$\text{Intensity of magnetization} = \frac{\text{Magnetic dipole moment}}{\text{Volume}}$$

$$I = \frac{M}{V} \qquad \ldots(3.2)$$

The units of intensity of magnetization is

$$I = \frac{\text{ampere metre}^2}{\text{metre}^3} = \frac{\text{ampere}}{\text{metre}} \text{ or } Am^{-1}$$

Thus intensity of magnetization and magnetic intensity have same units.

If the magnetic specimen has area of cross section 'a' and length $2l$, then its volume is

$$\text{Volume } (V) = a \times 2l = 2al$$

If m is the pole strength developed, then magnetic dipole moment of the specimen is

$$M = m \times 2l = 2ml$$

$\therefore$ Intensity of magnetization

$$I = \frac{M}{V} = \frac{2ml}{2al} = \frac{m}{a} \qquad \ldots(3.3)$$

Hence intensity of magnetization is also defined as pole strength developed per unit area of cross-section of the speciman.

3. Magnetic Flux

Magnetic flux through a surface is defined as the number of magnetic lines of force passing normally through the surface. It is denoted by ϕ.

Consider a surface $\vec{dS}$ is held in a magnetic field of induction $\vec{B}$, then magnetic flux passing normally through the surface is given as

$$\phi = \vec{B}.\vec{dS} \qquad \ldots(3.4)$$

The S.I units of magnetic flux is Weber (Wb)

4. Magnetic Induction

Consider a soft iron piece placed in a uniform magnetic field B_0 set up in vacuum. The uniform magnetizing field B_0 is represented by paralle lines as shown in Fig. (3.1*a*). The iron piece get magnetized when placed in the magnetic field. This induced magnet will have north and south magnetic poles shown by N and S respectively. The induced magnet will produce its own magnetic field. In regions C and D since the magnetic lines of force are in the same direction as that of magnetizing field hence magnetizing field is strengthened while in regions A and G, the magnetizing field is opposed by the field produced by magnetization of soft iron bar. The resultant magnetic field is shown in Fig. (3.1*b*).

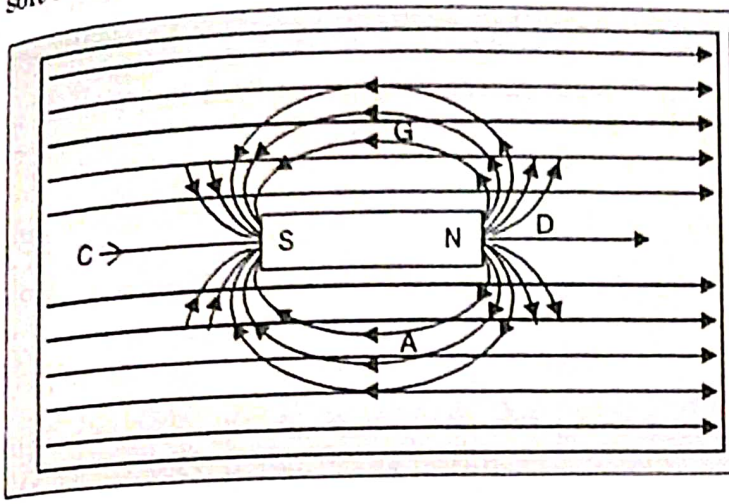


Fig. (3.1a)

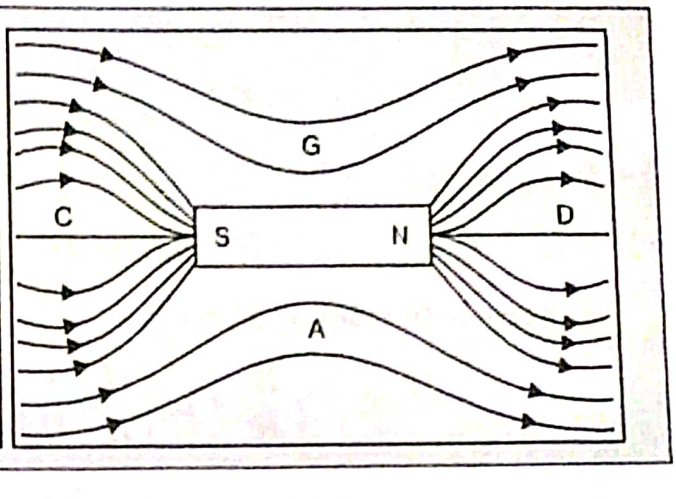


Fig. (3.1b)

Magnetic induction is defined as the number of magnetic lines of induction (magnetic field lines inside the material) crossing per unit area normally through magnetic material.

Thus magnetic induction B is the sum of magnetic field B_0 and magnetic field $\mu_0 I$ produced due to magnetization of the substance.

$$\therefore \quad B = B_0 + \mu_0 I$$

$$\text{or} \quad B = \mu_0 H + \mu_0 I \qquad (\because B_0 = \mu_0 H)$$

$$\text{or} \quad B = \mu_0 (H + I) \qquad \ldots(3.5)$$

Magnetic induction is also known as magnetic flux density or simply magnetic field.

The S.I. units of magnetic induction is tesla (T) or weber metre^{-2} ($Wb\ m^{-2}$).

Also $\quad 1 \text{ tesla} = 10^4 \text{ gauss}$

5. Magnetic Susceptibility

The magnetic susceptibility of a magnetic substane is defined as the ratio of intensity of magnetization to the magnetic intensity.

It is denoted by X_m

$$\therefore \quad X_m = \frac{I}{H} \qquad \ldots(3.6)$$

The magnetic susceptibility of a magnetic sustance gives a measure of its easiness to acquire magnetism. It has no units.

6. Magnetic Permeability

The magnetic permeability of a magnetic substance is defined as the ratio of the magnetic induction to the magnetic intensity.

It is denoted by μ

$$\therefore \quad \mu = \frac{B}{H} \qquad \ldots(3.7)$$

The magnetic permeability of a magnetic substance gives the measure of its conducting power towards the passage of magnetic lines of induction. Its S.I. unit is

$$\mu = \frac{\text{Tesla}}{\text{ampere metre}^{-1}} = \text{tesla metre ampere}^{-1} \ (TmA^{-1})$$

From eq. (3.5)

$$B = \mu_0 (H + I)$$

Dividing both sides by H, we get

$$\frac{B}{H} = \mu_0 \left(\frac{H}{H} + \frac{I}{H} \right)$$

or $$\mu = \mu_0 \left(1 + \frac{I}{H} \right) \qquad \left(\because \mu = \frac{B}{H} \right)$$

or $$\mu = \mu_0 (1 + \chi_m) \qquad \text{Using eq. (3.6)}$$

$$\frac{\mu}{\mu_0} = 1 + \chi_m$$

$$\mu_r = 1 + \chi_m \qquad \ldots(3.8)$$

where $\mu_r = \frac{\mu}{\mu_0}$ is the relative permeability of the magnetic substance.

3.2 ATOM AS A MAGNETIC DIPOLE (ORBITAL MAGNETIC MOMENT OF AN ELECTRON)

In an atom, electrons revolve around the nucleus in circular orbits, may be considered as small current loops. Due to this, an atom possesses magnetic dipole moment and hence behaves as a magnetic dipole.

Consider, an electron of mass m and charge e revolves in a circular orbit of radius r around the positive charged nucleus with uniform speed v in the anticlockwise direction as shown in Fig. (3.2).

Angular momentum of electron due to its orbital motion is :

$$L = mvr \qquad \ldots(3.9)$$

Let time period of orbital motion of electron = T. Thus in one second electron will cross any point on its orbit $\frac{1}{T}$ lines.

Thus orbital motion of electron is equivalent to current.

$$I = \frac{e}{T} \qquad \text{...(3.10) } \left(\text{Current} = \frac{\text{Charge}}{\text{Time}}\right)$$

Period of revolution of electron (i.e. time period) is given as

$$T = \frac{2\pi r}{\upsilon} \qquad \text{...(3.11)}$$

$\therefore$ Current $$I = \frac{e\upsilon}{2\pi r} \qquad \text{..(3.12) Using eq. (3.10)}$$

Area of electron orbit (i.e. area of current loop)

$$A = \pi r^2 \qquad \text{...(3.13)}$$

$\therefore$ Magnetic dipole moment of the atom is given as

$$M = IA \qquad \text{...(3.14)}$$

or $$M = \left(\frac{e\upsilon}{2\pi r}\right) \times \pi r^2 \qquad \text{[using eqs. (3.12 \& 3.13)}$$

or $$M = \frac{e\upsilon r}{2} \qquad \text{...(3.15)}$$

From eq. (3.9)

$$\upsilon r = \frac{L}{m}$$

Putting this value in eq. (3.15), we get

$$M = \left(\frac{e}{2m}\right) L \qquad \text{...(3.16)}$$

In vector form

$$\vec{M} = -\left(\frac{e}{2m}\right) \vec{L} \qquad \text{...(3.17)}$$

Where –ve sign is due to negative charge on electron.

Eq. (3.17) indicates that magnetic moment vector is directed in direction opposite to that of angular momentum vector.

According to Bohr's theory the angular momentum of electron in a stationary orbit is equal to integral multiple of $\frac{h}{2\pi}$ where h is Planck's constant

i.e. $$L = \frac{nh}{2\pi}$$

where $n = 1, 2, 3 \ldots$

Putting this value in eq. (3.16), we get

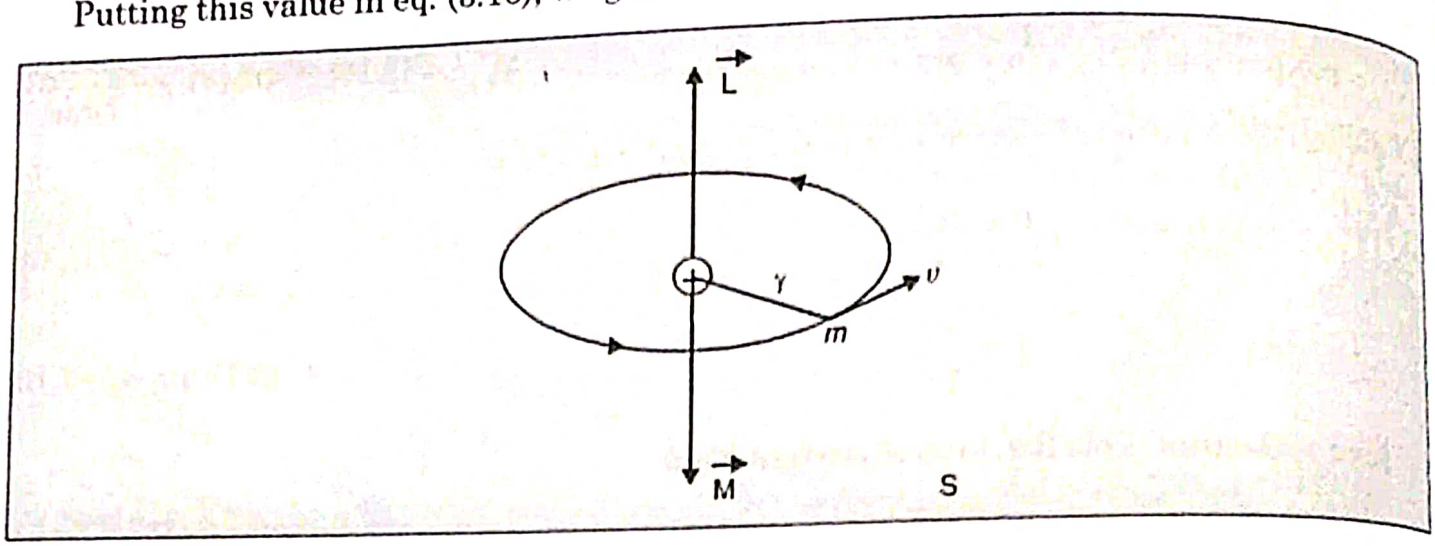


Fig. 3.2

$$M = \left(\frac{e}{2m}\right)\frac{nh}{2\pi}$$

Or $$M = n\left(\frac{eh}{4\pi m}\right) = n\left(\frac{e\hbar}{2m}\right) \quad \ldots(3.18) \text{ where } \hbar = \left(\frac{h}{2\pi}\right)$$

Thus eq. (3.18) gives magnetic moment of electron due to its orbital motion.

The minimum value of orbital magnetic moment of electron (for n = 1) is given as

$$M = \frac{e\hbar}{2m} = \frac{eh}{4\pi m} = \mu_B \text{ called Bohr magneton}$$

The numerical value of Bohr magneton

$$\mu_B = \frac{eh}{4\pi m} = \frac{(1.6\times10^{-19}\,C)\times(6.62\times10^{-34}\,J-s)}{4\times(3.14)\times(9.1\times10^{-31}\,kg)} = 9.27\times10^{-24}\,Am^2$$

In an atom, in addition to orbital motion, an electron has spin motion also. The electron possesses magnetic moment due to its spin motion also. The total magnetic moment of the electron is the vector sum of its magnetic moments due to orbital and spin motion.

3.3 DIA, PARA AND FERRO-MAGNETIC SUBSTANCES

The substances which get magnetized when placed in the magnetic field are called magnetic substances (materials). The magnetization develop in a substance may be parallel or antiparallel to the applied magnetic field. The response may be strong or weak. Depending upon the magnitude and sign of response to the applied magnetic field and also the effect of temperature on magnetic properties, the magnetic materials are mainly classified into following three categories.

(I) Diamagnetic materials (II) Paramagnetic materials and (III) Ferromagnetic materials.

(I) DIAMAGNETIC MATERIALS

The materials which when placed in a magnetic field become feebly (weakly) magnetized in a direction opposite to that of applied external magnetic field, are called diamagnetic materials. Examples of diameterials are :

Bismuth, antimony, gold, mercury, lead, quartz etc.

Properties : Following are the properties of diamagnetic materials.

(i) A diamagnetic substance is feebly repelled by a magnet. When a diamagnetic substance is placed in the magnetic field, its atoms acquire a small magnetic dipole moment in a direction opposite to the external applied magnetic field. As a result, the diamagnetic substance moves from stronger part of the magnetic field to its weaker part *i.e.* it is feebly repelled by magnet.

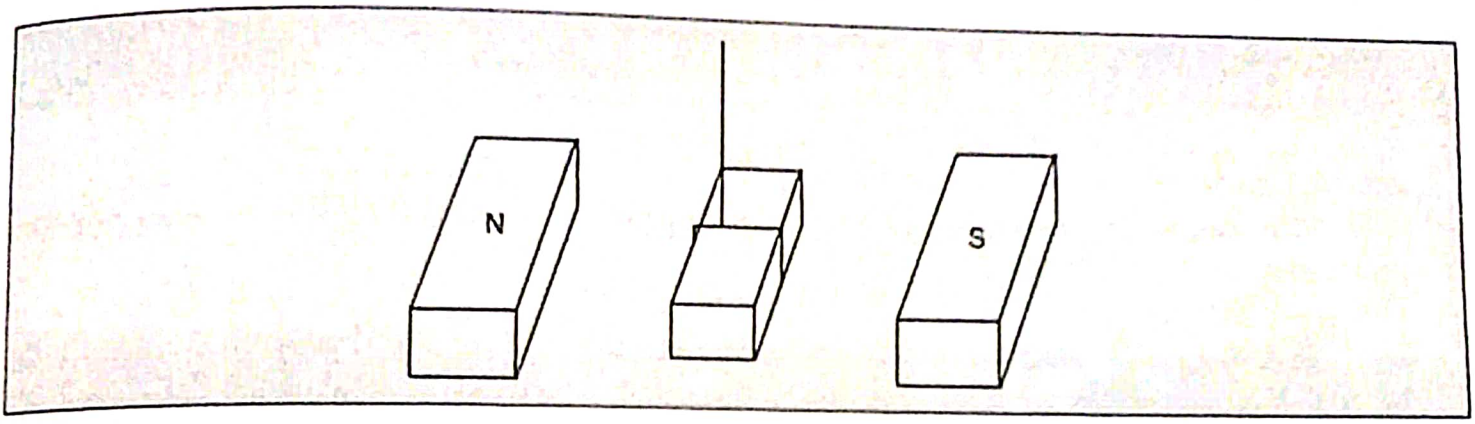


Fig. 3.3

(ii) When a rod of diamagnetic substance is suspended inside a magnetic field, it slowly sets itself at right angles to the direction of field as shown in Fig. (3.37). This is due to the fact that a diamagnetic substance is weakly repelled by a magnet.

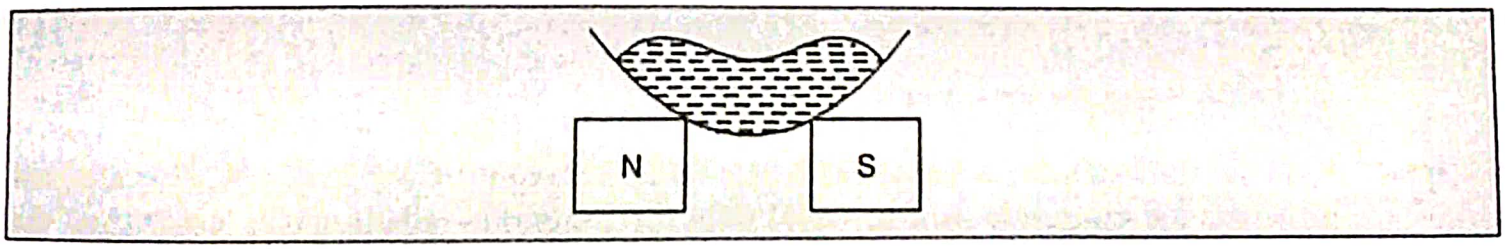


Fig. 3.4

(iii) If a diamagnetic liquid contained in a watch glass is placed on two closed spaced pole pieces of a magnet, it suffers a slight depression in the middle as shown in Fig. 3.4. However, the liquid shows a rise, in the middle, when pole, pieces are moved apart as shown in Fig. 3.5.

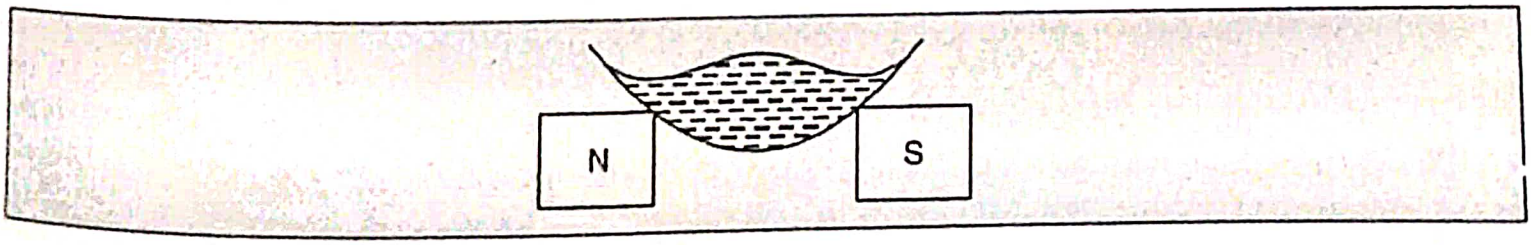


Fig. 3.5

(iv) For a diamagnetic substance, the intensity of magnetization (I) has a small negative value.

(v) When a diamagnetic material is placed inside a magnetic field the magnetic lines become slightly less dense in the magnetic material as shown in Fig. 3.6.

When a diamagnetic substance is placed in a magnetic field, a small magnetization occurs opposite to the direction of the field. Due to this reason, the magnetic field lines become less dense in the magnetic material.

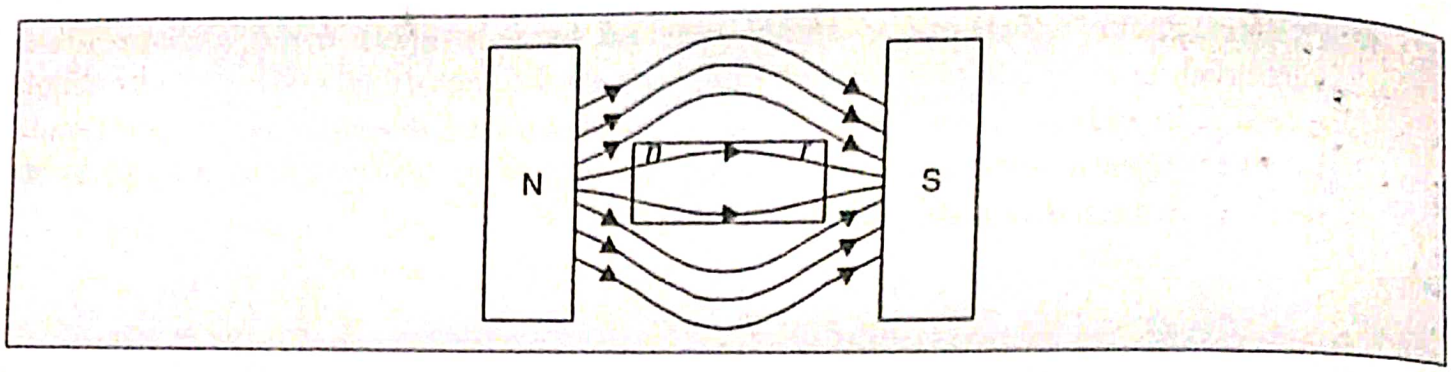


Fig. 3.6

(vi) The magnetic susceptibility (χ_m) of a diamagnetic substance has a small negative value.

Since $\chi_m = \frac{I}{H}$ and for a diamagnetic material, I has small negative value, hence χ_m will have a small negative value.

(vii) The relative permeability (μ_r) of a diamagnetic substance is slightly less than 1.

Since for a diamagnetic material, has a small negative value, therefore from relation.

$$\mu_r = 1 + \chi_m \qquad \ldots(3.18)$$

μ_r will be slightly less than 1.

(viii) When a diamagnetic substance is placed in a magnetizing field (H), the magnetic induction (or magnetic flux density) B in the magnetic substance is lesser than that in vacuum (μoH).

Since for a diamagnetic substance, I has a small negative value therefore from relation.

$$B = \mu_0 (H + I)$$

B will be less than μoH

(ix) The diamagnetic substance do not obey Curie's law.

(II) PARAMAGNETIC MATERIALS

The materials which when placed in a magnetic field, become weakly (feebly) magnetized, in the direction of applied magnetic field, are called paramagnetic materials. The examples of paramagnetic materials are platinum, aluminium, chromium, manganese etc.

Properties : Following are the properties of paramagnetic substances :

(i) A paramagnetic substance is feebly attracted by a magnet.

(ii) When a rod of paramagnetic substance is suspended inside a magnetic field, it slowly sets itself parallel to the direction of magnetic field as shown in Fig. 3.7. It happens because, a paramagnetic substance is weakly attracted by a magnet.

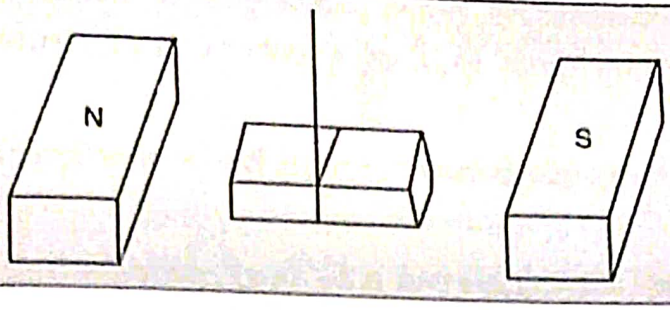


Fig. 3.7

(iii) If a paramagnetic liquid contained in a watch glass is placed on two closely spaced pole-pieces of a magnet, it shows a slight rise in the middle as shown in Fig. 3.8. When the poles are moved apart, the paramagnetic liquid gets depressed in the middle as shown in Fig. 3.9.

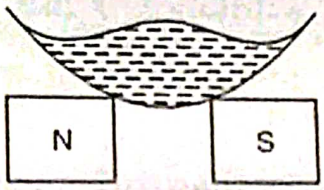


Fig. 3.8

(iv) For a paramagnetic substance the intensity of magnetization (I) has a small positive value.

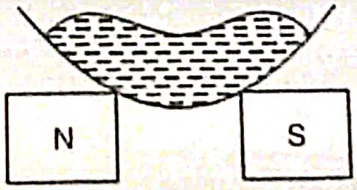


Fig. 3.9

(v) When a paramagnetic material is placed in the magnetic field, the magnetic lines become slightly dense in magnetic material as shown in Fig. 3.10.

(vi) The magnetic susceptibility (χ_m) of a paramagnetic substance has a small positive value.

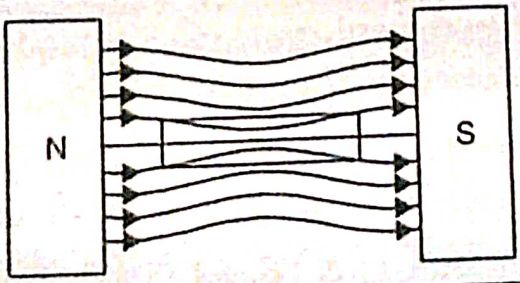


Fig. 3.10

Since for a paramagnetic substance, (I) has a small positive value, therefore from relation.

$$\chi_m = \frac{I}{H} \quad ...(3.19)$$

χ_m has small positive value.

(vii) The relative permeability (μ_r) of a paramagnetic substance is slightly greater than 1.

Since for a paramagnetic substance, χ_m has a small positive value, therefore from relation.

$$\mu_r = 1 + \chi_m \quad ...(3.20)$$

μ_r will be slightly greater than 1.

(viii) When a paramagnetic substance is placed inside a magnetizing field (H), the magnetic flux density (B) in the paramagnetic substance is greater than that in vacuum ($\mu_0 H$).

Since for a paramagnetic substance, I has a small positive value, hence from relation.

$$B = \mu_0 (H + I)$$

It follows that B will be greater than $\mu_0 H$.

(ix) The paramagnetic substances obey Curie law i.e. the susceptibility of a paramagnetic substance is inversely proportional to its absolute temperature.

$$\chi_m \propto \frac{1}{T} \quad ...(3.21)$$

It follows that a paramagnetic substance tends to lose its magnetic character on being heated.

(III) FERROMAGNETIC MATERIALS

Those materials, which when placed in a magnetic field are strongly magnetized in the direction of the applied magnetic field are called ferromagnetic substances. The examples of ferromagnetic materials are iron, nickel, cobalt, gadolinium and other alloys.

Properties : Properties of ferromagnetic materials are as given below :

(i) A ferromagnetic substance is strongly attracted by a magnet.

(ii) When a rod of ferromagnetic substance is suspended in a magnetic field, it quickly aligns itself along the direction of magnetic field.

(iii) The ferromagnetic materials move from weaker part of the magnetic field to the stronger part, when placed in a magnetic field.

(iv) When a ferromagnetic material is placed inside a magnetic field, the magnetic field lines become highly dense in the ferromagnetic substance.

(v) For a ferromagnetic substance, the intensity of magnetization (I) has a large positive value.

(vi) The magnetic susceptibility (χ_m) of a ferromagnetic substance has a large positive value.

It follows from relation

$$\chi_m = \frac{I}{H} \qquad \ldots(3.22)$$

Since for a ferromagnetic substance, I has a large positive value, hence value of χ_m is also large positive value.

(vii) The relative permeability (μ_r) of a ferromagnetic substance is extremely large as compared to 1.

It follows from relation

$$\mu_r = 1 + \chi_m$$

Since χ_m has a large positive value, hence μ_r also has large positive value.

(viii) When a ferromagnetic substance is placed inside the magnet field (H), the magnetic induction (B) in the ferromagnetic substance is much larger than that in vacuum ($\mu_0 H$)

It follows from the relation

$$B = \mu_0 (H + I) \qquad \ldots(3.23)$$

Since I has large positive value, hence B is much larger than (μ_0H)

(ix) The ferromagnetic substances do not obey Curie law.

3.4 ATOMIC THEORY OF MAGNETISM (QUALITATIVE)

We know that atom behaves as magnetic dipole. The magnetic dipole moment of an atom is equal to the vector sum of orbital and spin magnetic moment of the unpaird electrons in the outermost shell.

(I) Paramagnetism

In paramagnetic materials, each molecule contains one or more unpaired electrons. The dipole moment of the electrons except the last unpaired electron cancel each other. Thus the magnetic moment of the atom or molecule, due to last unpaired electron, is non zero in obsence of external magnetic field However due to the thermal agitations at room temperature, various dipoles in the sample are randomly oriented. Hence overall magnetic dipole moment of the paramagnetic sample is zero when there is no external applied magnetic field.

When external magnetic field is applied across the sample the each magnetic dipole experiences tonque due to which dipoles tends to align in the direction of external magnetic field. Hence net magnetic dipole moment of the sample becomes non zero as more dipoles are ordered in the direction of magnetic field. This explains paramagnetism. Further with

increase in magnitude of external magnetic field, more depoles are aligned in the direction of magnetic field. On the other hand with increase in temperature, dipoles get theremal excitation, which provide randomness to the already aligned dipoles. Thus magnetic susceptibility of these materials decreases with increase of temperature.

(ii) Diamagnetism

This effect is observed predominantly in those substances, whose atoms or molecules contain even number of electrons. Thus net magnetic dipole moment of each molecule or atom is zero under natural conditions. When external magnetic field is applied across such material then no torque is experienced by atomic dipoles, but the external magnetic field modifies the electronic motion within each atom. The orbit of each electron behaves as current loop and produces its own magnetic field. Those electrons, whose current loop is so oriented that its magnetic field is in direction similar to the external field get slowed down, while electrons whose loops are so oriented that their own magnetic field is opposite to the external magnetic field, get accelerated due to Lenz's law. Thus every electron pair within same orbit acquires a net magnetic dipole moment in a direction opposite to external magnetic field. This explains diamagnetism. Thermal agitations does not effect this mechanism. Hence their magnetic susceptibility is independent of the temperature.

(iii) Ferromagnetism

In ferromagnetic-substances the atomic dipoles of sample exist in groups, called domains. In one domain the direction of all diples is same but is different from the direction of dipoles in other domain. The linear dimensions of each domain can be upto 1000 A°. In the absence of external magnetic field, the dipole moments of the domains are randomly oriented, so as to form closed loops so that net dipole moment of the sample is zero as shown in Fig. (3.11).

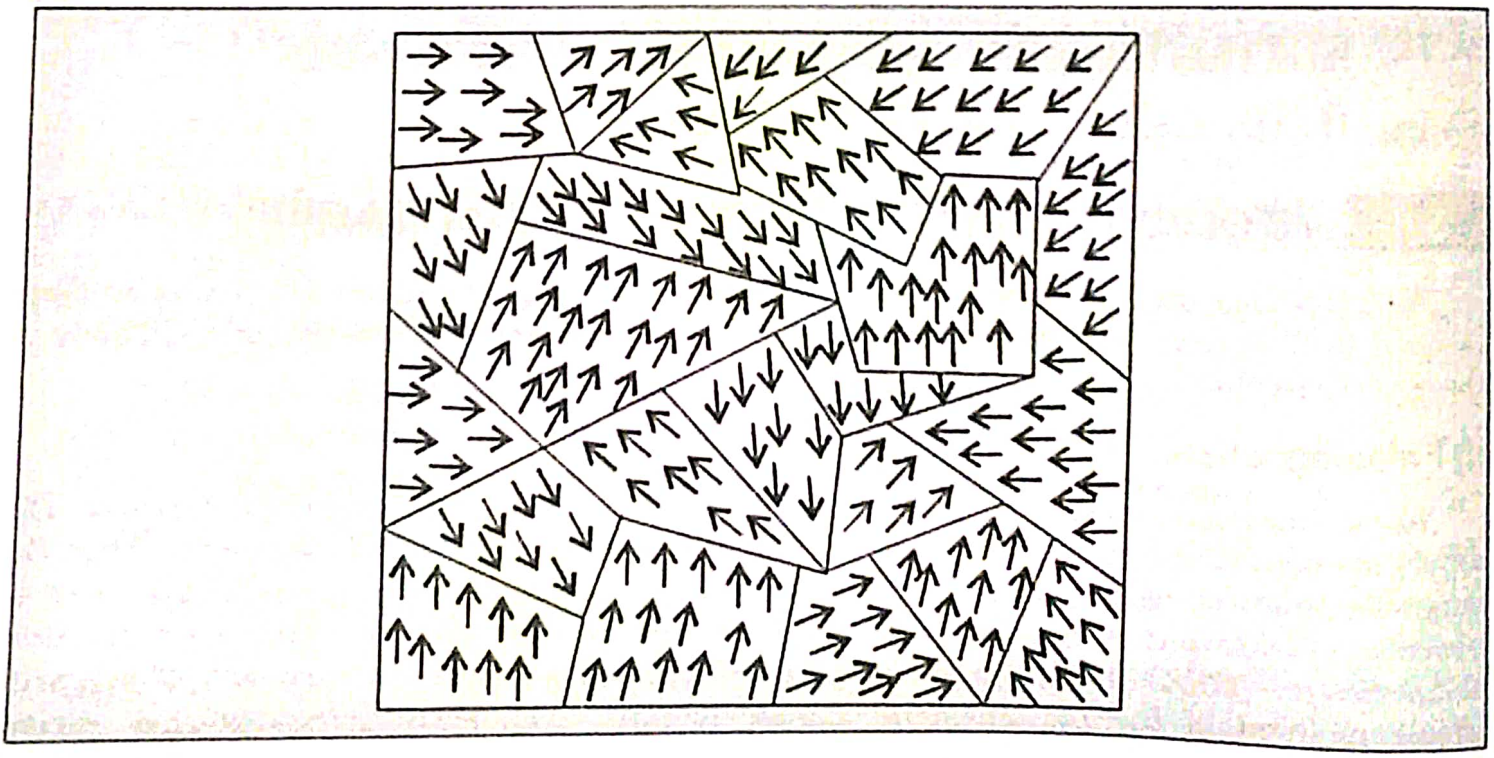


Fig. 3.11

When material is placed in external magnetic field then domains which are favourably magnetized in the direction of magnetic field, grow in size while the other domains reduce in size. As a result the material is rapidly magnetized in the direction of external magnetic field.

If material the external magnetic field is strong enough, then the domain may rotate as a single entity so as to align its magnetic dipole moment in the direction of external magnetic field. When external magnetic field is removed then the domains do not move back to their original position. Thus material becomes permanent magnet. This explains ferromagnetism. If temperature is increased it may repture magnetic domains and material behaves like paramagnetic substance.

3.5 CLASSICAL LANGEVIN THEORY OF DIAMAGNETISM

Diamagnetism is observed in all those substances in which atoms have even number of electrons around the nucleus. According to this theory, the diamagnetism could be traced to the orbital motion of the electrons.

For simplicity consider an atom having two electrons around the nucleus. These two electrons move around the nucleus with the same speed on like orbits but in opposite directions as shown in Fig. (3.12 ab). The oribital magnetic moment of one electron is equal but opposite to the orbital magnetic moment of the second electron. Hence total magnetic moment of the atom is zero. In other words diamagnetic substance has zero magnetic moment.

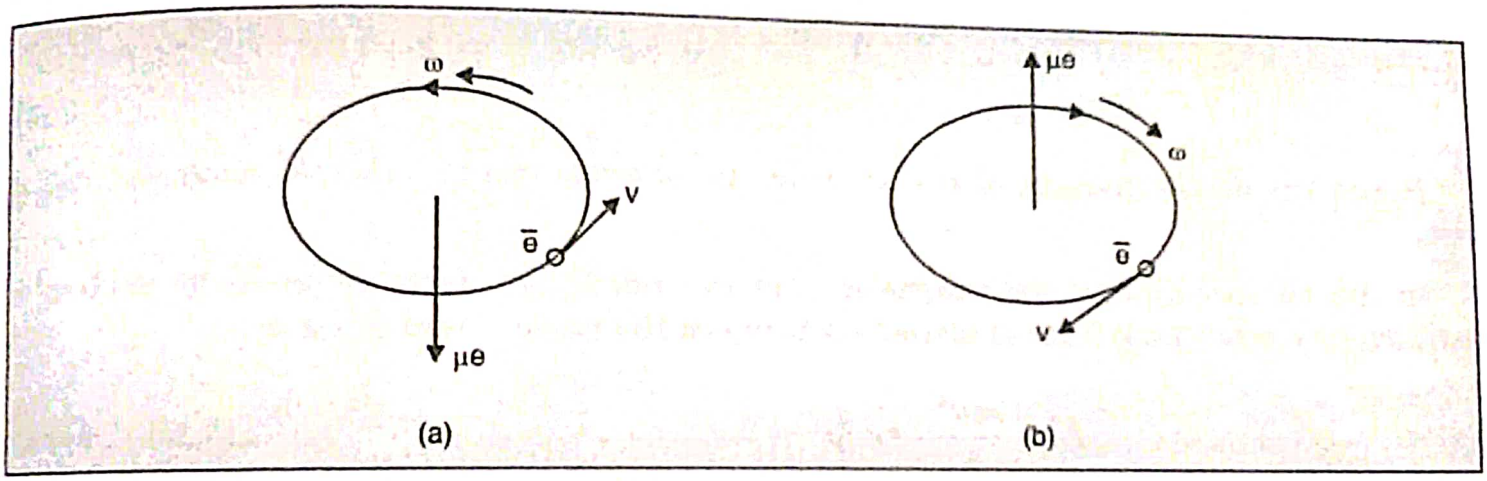


Fig. 3.12

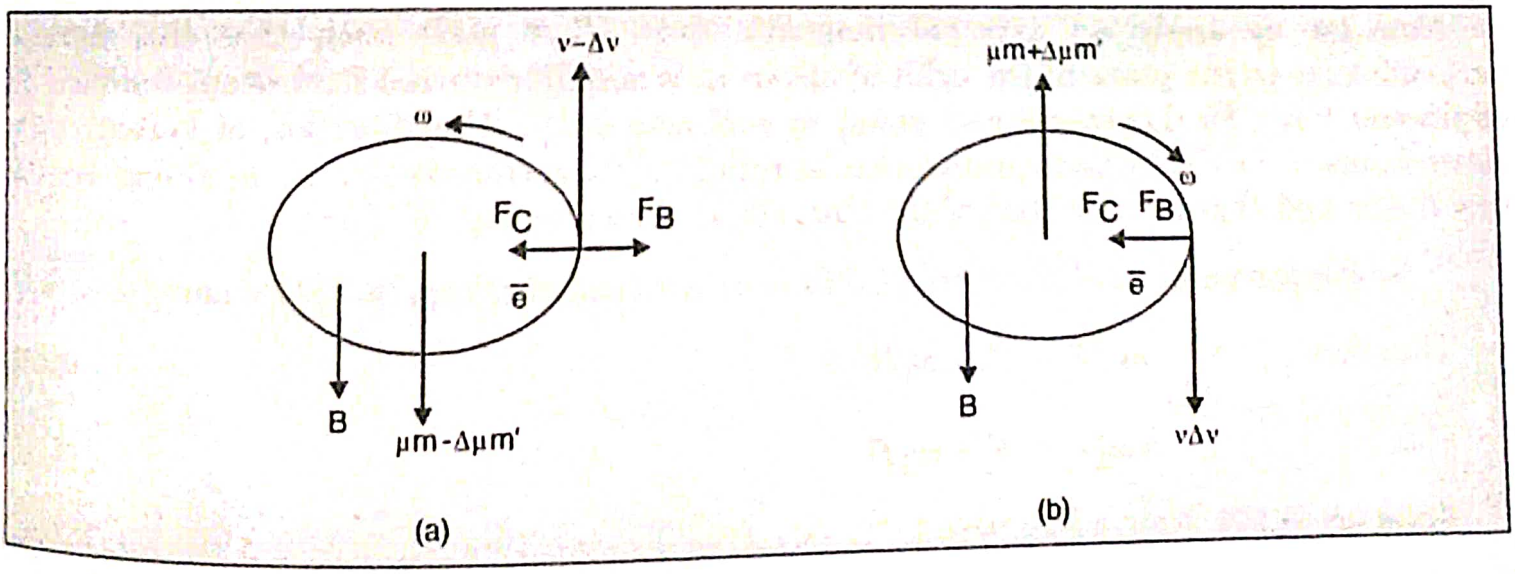


Fig. 3.13

Let i is the electronic current and r radius of orbit (assumed to be circular), then magnetic dipole moment of each electron is given as

Magnetic moment of each electron = $I(A)$

$$= I\,(\pi r)^2$$

$$= \left(\frac{e}{T}\right)\pi r^2$$

$$= \left(\frac{e}{\left(\frac{2\pi}{\omega_0}\right)}\right)(\pi r^2) \qquad \left(\because T = \frac{2\pi}{\omega_0}\right)$$

$$= \frac{1}{2}e\omega_0^2 r \qquad \ldots(3.24)$$

Where ω_0 is angular velocity of each electron.

Therefore net magnetic moment of the atom

$$\mu_m = \frac{1}{2}e\omega_0^2 r - \frac{1}{2}e\omega_0^2 r$$

$$\therefore\ \mu_m = 0 \qquad \ldots(3.25)$$

Hence net dipole moment of the atom in the absence of any external magnetic field is zero.

In the absence of external magnetic field the centripetal force required by electron is provided by electrostatic force of attraction between the nucleus and electron.

$$F_c = \frac{mv^2}{r} = m\omega_0^2 r \qquad ..(3.26)\ (\because v = r\omega)$$

The direction of centripetal force is towards centre of the orbit.

Now let us apply an external magnetic field ($B = \mu_0 H$) such that this field is perpendicular to the plane of the orbit of electron. When an external field is applied then an additional force F_B (Lorentz force) equal to evB acts on it. The direction of Lorentz force depends upon the clockwise or anticlockwise rotation of electron. Let v_1, v_2, ω_1 and ω_2 are the new linear and angular velocities of the electron as shown in Fig. (3.13ab).

$\therefore$ New centripetal force = Centripetal force in absence of magnetic field ± Lorentz force

Therefore $$m\omega_1^2 r = F_c - ev_1 B \qquad \ldots(3.27)$$

and $$m\omega_2^2 r = F_c + ev_2 B \qquad \ldots(3.28)$$

From eq. (3.27)

$$m\omega_1^2 r = F_c - ev_1 B$$

or $$m\omega_1^2 r = m\omega_0^2 r - ev_1 B$$ using eq. (3.26)

or $$m\omega_1^2 r = m\omega_0^2 r - e\omega_1 rB \qquad (\because v_1 = r\omega_1)$$

or $$m\omega_1^2 = m\omega_0^2 - e\omega_1 B$$

or $$\omega_1^2 = \omega_0^2 - \frac{e\omega_1 B}{m} \qquad \ldots(3.29)$$

From eq. (3.28)

$$m\omega_2^2 r = F_c + ev_2 B$$

or $$m\omega_2^2 r = m\omega_0^2 r + ev_2 B \qquad \text{using eq. (3.26)}$$

or $$m\omega_2^2 r = m\omega_0^2 r + er\omega_2 B \qquad (\because v_2 = r\omega_2)$$

or $$m\omega_2^2 = m\omega_0^2 + e\omega_2 B$$

or $$\omega_2^2 = \omega_0^2 + \frac{e\omega_2 B}{m} \qquad \ldots(3.30)$$

Subtracting eq. (3.30) from eq. (3.29), we get

$$\omega_1^2 - \omega_2^2 = -\frac{eB}{m}(\omega_1 + \omega_2)$$

or $$(\omega_1 - \omega_2)(\omega_1 + \omega_2) = -\frac{eB}{m}(\omega_1 + \omega_2)$$

or $$\omega_1 - \omega_2 = -\frac{eB}{m}$$

or $$\Delta\omega = -\frac{eB}{m} \qquad ..(3.31)$$

Magnetic moment of electron is given by

$$\mu_m = IA = \frac{e}{T} \times \pi r^2$$

$$= \frac{e}{\left(\frac{2\pi}{w}\right)}(\pi r^2) \qquad \left(\because T = \frac{2\pi}{\omega}\right)$$

$\therefore$ $$\mu_m = \frac{e\omega r^2}{2} \qquad \ldots(3.32)$$

and change in magnetic moment due to change in ω i.e.

i.e. $$\Delta\mu_m = \frac{e}{2}\Delta\omega r^2$$

or $$\Delta\mu_m = -\frac{e}{2}\left(\frac{eB}{m}\right)r^2$$ using eq. (3.31)

$$\Delta\mu_m = -\frac{Be^2r^2}{2m} \quad \ldots(3.33)$$

This change is actually the relative change in dipole moment of two electrons due to change in their angular velocity.

If $\Delta\mu_{m'}$ is the change in dipole moment of each electron, then

$$\Delta\mu m = \Delta\mu_{m'} - (-\Delta\mu_{m'})$$

$$\Delta\mu_m = \Delta\mu_{m'} + \Delta\mu_{m'}$$

$$\Delta\mu_m = 2\Delta\mu_{m'}$$

$$\therefore \quad \Delta\mu_{m'} = \frac{\Delta\mu_m}{2}$$

or $$\Delta\mu_{m'} = -\frac{Be^2r^2}{4m} \quad \ldots(3.34)\ [\text{using eq. (3.33)}]$$

or $$\Delta\mu_{m'} = -\frac{\mu_0 e^2 r^2}{4m}H \quad \ldots(3.35)\ (\because B=\mu_0 H)$$

When applied to an atom, eq. (3.35) needs modification, because the electrons revolve around spherical surface rather than a circular one i.e. the diamagnetic atom has a spherical symmetry. Also, if the electronic orbits are not perpendicular to the applied magnetic field, then r is replaced by r_1 the projection of the radius r of the orbit on the plane perpendicular to the magnetic field.

$$\therefore \quad \Delta\mu_{m'} = -\frac{\mu_0 e^2 r_1^2}{4m}H \quad \ldots(3.36)$$

If now we consider the induced magnetic moment of whole of the atom, instead of an electron, then $$\mu = \Sigma\Delta\mu m' = -\frac{\mu_0 e^2 H}{4m}\Sigma r_1^2 \quad \ldots(3.37)$$

If x, y and z are the co-ordinates of radius r of the orbit, then

$$r^2 = x^2 + y^2 + z^2$$

For spherical symmetry

$$x^2 = y^2 = z^2 = \frac{r^2}{3} \quad \ldots(3.38)$$

Further, if the z axis is chosen to be in the plane perpendicular to the applied magnetic field, then

$$r_1^2 = x^2 + y^2$$

or $$r_1^2 = \frac{r^2}{3} + \frac{r^2}{3} = \frac{2r^2}{3}$$ using eq. (3.38)

Putting this value in eq. (3.37), we get

$$\mu = \Sigma \Delta\mu_{m'} = -\frac{\mu_0 e^2 H}{4m} \times \frac{2}{3} \Sigma r^2$$

$$\mu = -\frac{\mu_0 e^2 H}{6m} \Sigma r^2 \quad ...(3.39)$$

If there are n atoms per unit volume and Z is the atomic number of atoms, then intensity of magnetization (I) is given by

$$I = nZ\mu$$

$$I = -\frac{nZ\mu_0 e^2 H}{6m} \Sigma r^2 \quad ...(3.40)$$

Hence diamagnetic susceptibility

$$\chi_m = \frac{I}{H}$$

$$\chi_m = -\frac{nZ\mu_0 e^2}{6m} \Sigma r^2 \quad ..(3.41)$$

From eq. (3.41), it is clear that the magnetic susceptibility is independent of temperature. Hence Curie's law (i.e. $\chi \propto \frac{1}{T}$) is not obeyed by diamagnetic substances.

3.6 LANGEVIN THEORY OF PARAMAGNETISM

The orbital and spin motion of electrons around the nucleus of an atom give rise to magnetic dipole moment. In a paramagnetic substance, each atom has a permanent magnetic moment, but the magnetic moments are randomly oriented in the absence of external magnetic field. The net magnetic moment is zero. When external magnetic field is applied, these permanent magnetic dipoles align parallel to applied magnetic field. The magnetization depends upon the following two factors.

(i) **The applied magnetic field.** The applied magnetic field tends to align the magnetic axes of the molecules in its own direction.

(ii) **The thermal agitation.** The thermal agitation disorganise the orderly state produced by applied magnetic field.

At any given temperature, a statistical equilibrium is reached. Now, majority of molecules have their axes parallel to the field direction and thus contribute to intensity of magnetization.

Langevin gave a theoretical interpretation of paramagnetism on the basis of the kinetic

theory of gas and obtained a quantitative relation for the paramagnetic gas which justify experimental result of curie.

Consider unit volume of a paramagnetic sample having N number of atoms. If the magnetic dipole moment of each dipole is $\vec{\mu}_m$ and angle θ between $\vec{B}$ and $\vec{\mu}_m$ as shown in Fig. 3.14.

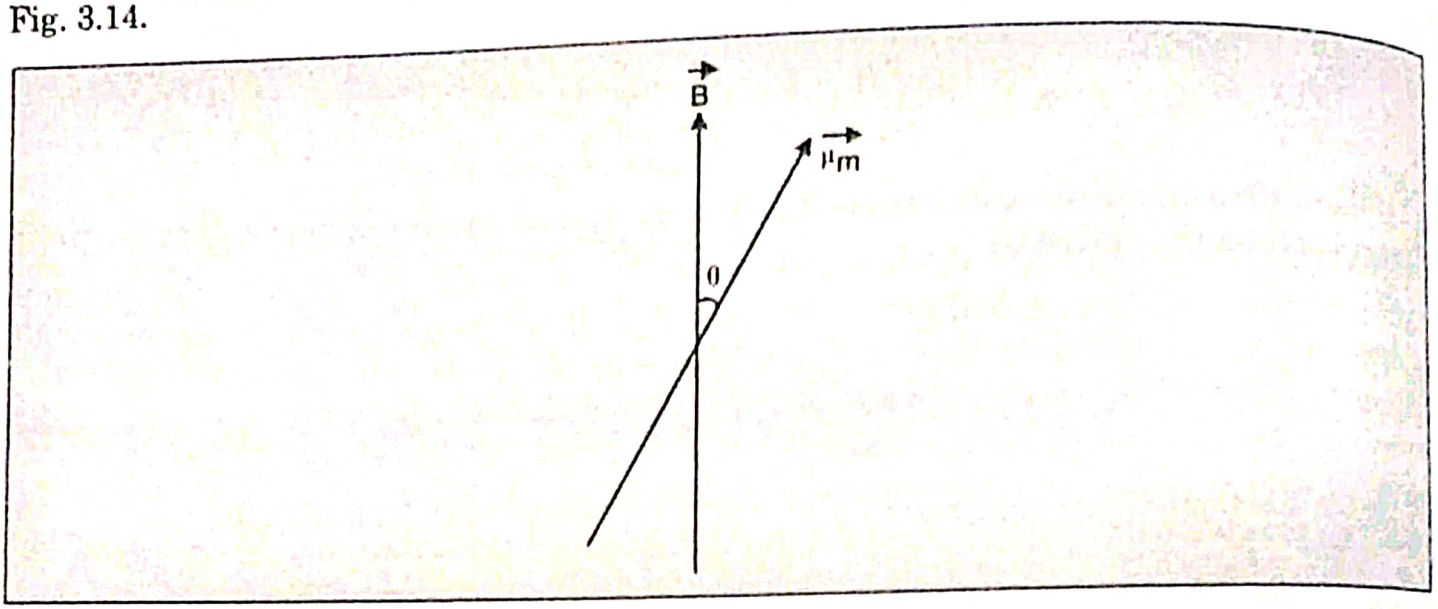


Fig. (3.14)

Torque acting on the dipole is

$$\vec{\tau} = \vec{\mu}_m \times \vec{B}$$

or
$$\tau = \mu_m B \sin\theta \qquad \ldots(3.42)$$

Small amount of work done by external agency in displacing the dipole through an angle $d\theta$ is.

$$dW = \tau d\theta = \mu_m B \sin\theta \, d\theta$$

Total work done in displacing the dipole from $\theta = 0$ to $\theta = \theta$ is given by

$$W = \int dW = \int_0^{\theta} \mu_m B \sin\theta d\theta$$

$$\Rightarrow \qquad W = \mu_m B \int_0^{\theta} \sin\theta d\theta = -\mu_m B \cos\theta$$

This work done is stored in the form of magnetic potential energy (U)

$$\therefore \qquad U = -\mu_m B \cos\theta \qquad \ldots(3.43)$$

According to Maxwell Boltzmann law, the number of dipoles per unit volume within a solid angle $d\Omega$ and whose energy is U given by

$$dN = Ae^{-U/kT} d\Omega \qquad \ldots(3.44)$$

where k is Boltzmann constant.

A is constant of proportionality and T is absolute temperature.

$d\Omega$ is solid angle subtended by the shaded area at O as shown in Fig. (A)

Now
$$d\Omega = \frac{\text{Area of ring between } 0 \text{ and } 0+d\theta}{r^2}$$

$$d\Omega = \frac{2\pi(r\sin\theta)(rd\theta)}{r^2} = 2\pi\sin\theta d\theta \qquad ...(3.45)$$

Putting this value in eq. (3.44), we get

$$dN = A \times 2\pi\sin\theta e^{-U/kT} d\theta$$

$$= 2\pi A e^{-U/kT}\sin\theta d\theta \qquad ...(3.46)$$

$$dN = Ce^{-U/kT}\sin\theta d\theta \qquad ...(3.46)$$

where
$$C = 2\pi A$$

or
$$dN = Ce^{\mu_m B\cos\theta/kT}\sin\theta d\theta$$

or
$$dN = Ce^{x\cos\theta}\sin\theta d\theta \qquad ...(3.48)$$

where
$$x = \frac{\mu_m B}{kT} \qquad ...(3.49)$$

The component of dipole moment in the direction of magnetic field = $\mu_m \cos\theta$.

Therefore total magnetic moment per unit volume is given as

$$dp_m = dN \times \mu_m \cos\theta$$

or
$$dp_m = (Ce^{x\cos\theta}\sin\theta d\theta)\mu_m\cos\theta \qquad \text{using eq. (3.48)}$$

$$dp_m = Ce^{x\cos\theta}\mu_m\sin\theta\cos\theta d\theta$$

∴ Net dipole moment of all the dipoles per unit volume is given by

$$p_m = \int_0^{\pi} Ce^{x\cos\theta}\mu_m\sin\theta\cos\theta d\theta \qquad ...(3.50)$$

As all the orientations are confined between 0 and π, hence total number of atoms in the sample are :

$$N = \int_0^{\pi} dN = \int_0^{\pi} Ce^{x\cos\theta}\sin\theta d\theta \qquad ..(3.51)$$

Therefore, average dipole moment per unit atom in the direction of magnetic field is

$$\bar{\mu}_m = \frac{p_m}{N}$$

or
$$\bar{\mu}_m = \frac{\int_0^{\pi} C e^{x\cos\theta} \mu_m \sin\theta\cos\theta\, d\theta}{\int_0^{\pi} C e^{x\cos\theta} \sin\theta\, d\theta} \quad \text{[using eqs. (3.50 \& 3.51)]}$$

$$= \frac{C\mu_m \int_0^{\pi} e^{x\cos\theta} \sin\theta\cos\theta\, d\theta}{C\int_0^{\pi} e^{x\cos\theta} \sin\theta\, d\theta}$$

$$\bar{\mu}_m = \frac{\mu_m \int_0^{\pi} e^{x\cos\theta} \sin\theta\cos\theta\, d\theta}{\int_0^{\pi} e^{x\cos\theta} \sin\theta\, d\theta} \quad \ldots(3.52)$$

Put $\cos\theta = u$, then $-\sin\theta d\theta = du$

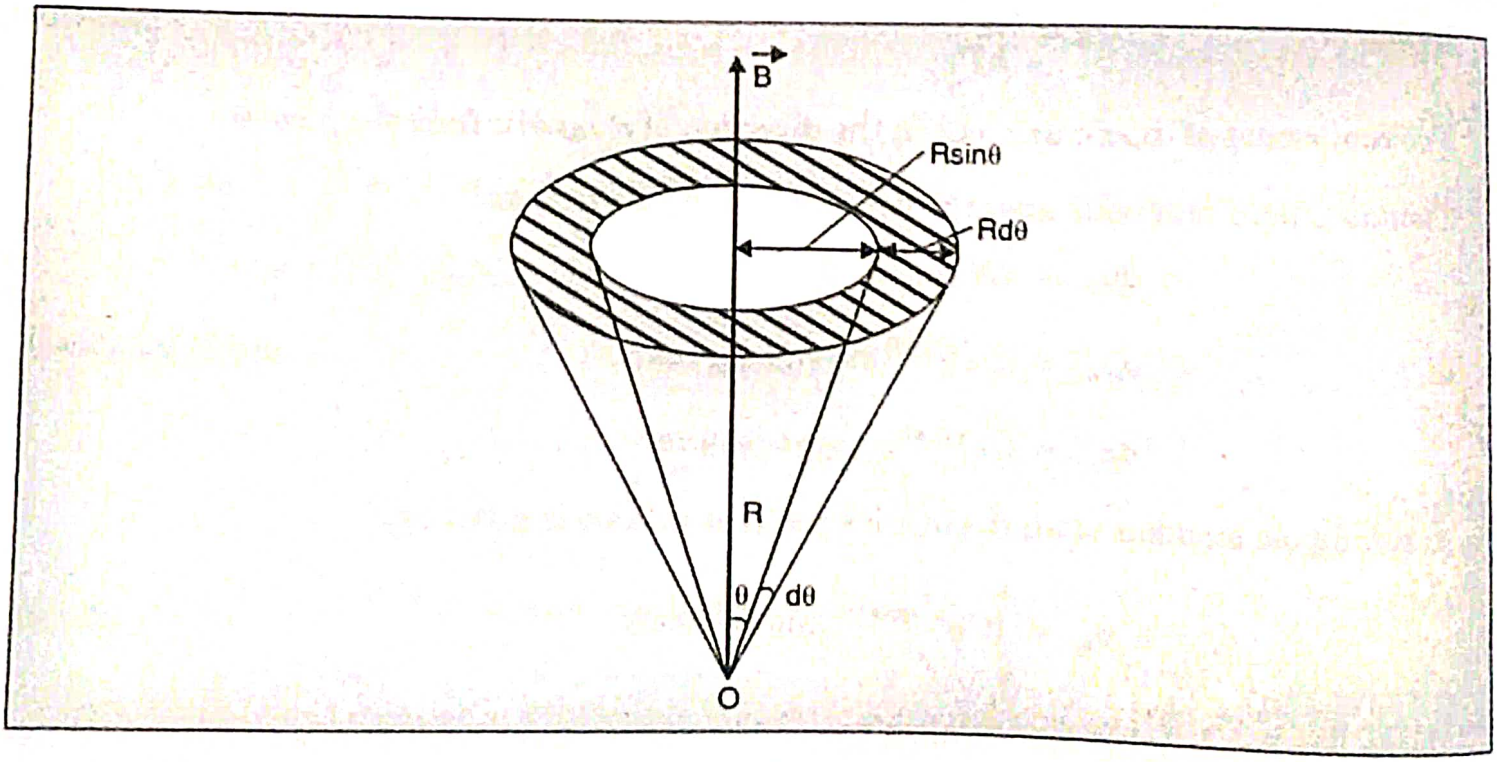


Fig. (A)

When $\theta = 0°$, then $u = \cos\theta = \cos 0 = 1$

When $\theta = \pi$, then $u = \cos\theta = \cos\pi = -1$

Putting these values in eq. (3.52), we get

$$\bar{\mu}_m = \frac{-\mu_m \int_1^{-1} u e^{xu} du}{-\int_1^{-1} e^{xu} du} = \frac{\mu_m \int_1^{-1} u e^{xu} du}{\int_1^{-1} e^{xu} du}$$

$$= \frac{\mu_m \left[\frac{1}{x}(e^x + e^{-x}) - \frac{1}{x^2}(e^x - e^{-x})\right]}{\frac{1}{x}(e^x - e^{-x})}$$

$$= \frac{\mu_m \left[\frac{\cosh x}{x} - \frac{\sinh x}{x^2}\right]}{\left(\frac{\sinh x}{x}\right)}$$

$$= \mu_m \left[\frac{\cosh x}{\sinh x} - \frac{1}{x}\right]$$

$$= \mu_m \left[\coth x - \frac{1}{x}\right]$$

The intensity of magnetization produced in the sample is given as

$$I = N\bar{\mu}_m$$

or $$I = N\mu_m \left(\coth x - \frac{1}{x}\right) \quad \ldots(3.52)$$

or $$I = N\mu_m L(x) \quad \ldots(3.53)$$

Where $L(x) = \left(\coth x - \frac{1}{x}\right)$ is called Langevin's function.

Special Cases

Case (i) : When $\mu_m B >> kT$ then $x = \frac{\mu_m B}{kT} >> 1$

(i.e. x is very large). In this case either T is small or B is large. Then

$$[L(x)]_{x\to\infty} = \left[\left(\coth x - \frac{1}{x}\right)\right]_{x\to\infty}$$

$$= \left[\frac{e^x + e^{-x}}{e^x - e^{-x}} - \frac{1}{x}\right]_{x\to\infty}$$

$$= \left[\frac{1+e^{-2x}}{1-e^{-2x}} - \frac{1}{x}\right]_{x\to\infty}$$

$$= \left[\frac{1+0}{1-0} - 0\right] = 1$$

Putting this value in eq. (3.53), we get

$$I = N\mu_m \quad \ldots(3.54)$$

Or

$$I = Is \quad \ldots(3.55)$$

Where Is is the saturation value of intensity of magnetization. This is the condition when all dipoles are completely aligned in the field direction.

Case (ii) : When $\mu_m B << kT$, then $x = \frac{\mu_m B}{kT} << 1$ (i.e. x is very small). In this case either T is large or B is small. Then $L(x)$ can be approximated as

$$L(x) \approx \cosh x - \frac{1}{x} = \left[\frac{1}{x} + \frac{x}{3} - \frac{x^2}{45} + \frac{2x^5}{945} + \ldots.\right] - \frac{1}{x}.$$

Neglecting x^2 and higher powers being very small

$$\therefore\ L(x) \approx \frac{1}{x} + \frac{x}{3} - \frac{1}{x} = \frac{x}{3} = \frac{\mu_m B}{3kT}$$

Putting this value in eq. (3.53), we get

$$I = \frac{N\mu_m^2 B}{3kT} \quad \ldots(3.56)$$

For a paramagnetic material I is very small

$$\therefore \quad B = \mu_0 (H + I)$$

$$B \approx \mu_0 H$$

Putting this value in eq. (3.56), we get

$$I = \frac{N\mu_m^2 \mu_0 H}{3kT} \quad \ldots(3.57)$$

$\therefore$ Magnetic susceptibility of a paramagnetic material

$$\chi_m = \frac{I}{H} = \frac{N\mu_0\mu_m^2}{3kT} \quad \ldots(3.58)$$

or

$$\chi_m = \frac{C'}{T}$$

where $C' = \frac{N\mu_0\mu_m^2}{3k}$ is called Curie's constant.

Eq. (3.58) shows that magnetic susceptibility of paramagnetic material is positive and varies inversely as absolute temperature. This is Curie's law.

3.7 CURIE'S LAW

According to this law, magnetic susceptibility (χ_m) is inversely proportional to the absolute temperature of the material.

It has been experimentally observed by Curie that intensity of magnetization ($\vec{I}$) of the magnetic material as (i) directly proportional to the magnetic field ($\vec{B}$) and (ii) inversely proportional to absolute temperature (T) of the material.

i.e. $$I \propto \frac{B}{T}$$

Since $B \propto H$

$\therefore$ $$I \propto \frac{H}{T}$$

or $$\frac{I}{H} \propto \frac{1}{T}$$

Since magnetic susceptibility

$$\chi_m = \frac{I}{H}$$

$\therefore$ $$\chi_m \propto \frac{1}{T} \qquad \ldots(3.59)$$

which is Curie's law.

According to law, the magnetic material gets magnetized easily if its temperature is low.

Curie Temperature. The temperature at which a ferromagnetic substance becomes paramagnetic substance is known as Curie temperature. Thus, ferromagnetic substance becomes paramagnetic substance if its temperature becomes more than the Curie temperature.

3.8 DOMAIN THEORY OF FERROMAGNETISM

Ferromagnetic materials show all the properties of paramagnetic materials but to a larger degree. Like paramagnetic substances, the atoms of ferromagnetic substances have a permanent magnetic moments. But in case of ferromagnetic substances the magnetic moments of individual atoms are coupled to the neigbhouring magnetic moments very strongly through **exchange interactions.** The large number of magnetic dipoles get aligned in the same direction, form large number of small effective regions called 'domains'. These domains are supposed to exist throughout the magnetic material as shown in Fig. (3.15). Each domain has a volume of the order of 10^{-2} cm^3 to 10^{-6} cm^3 and may contain about 10^{16} or more atomic dipoles. Each domain is magnetized to the degree of saturation in one direction.

The overall magnetization of ferromagnetic specimen is given by sum of domain vectors. However in normal state of the substance (i.e. when external magnetic field is absent) the different domains are randomly distributed. Hence their resultant magnetic moment is zero as shown in Fig. (3.16).

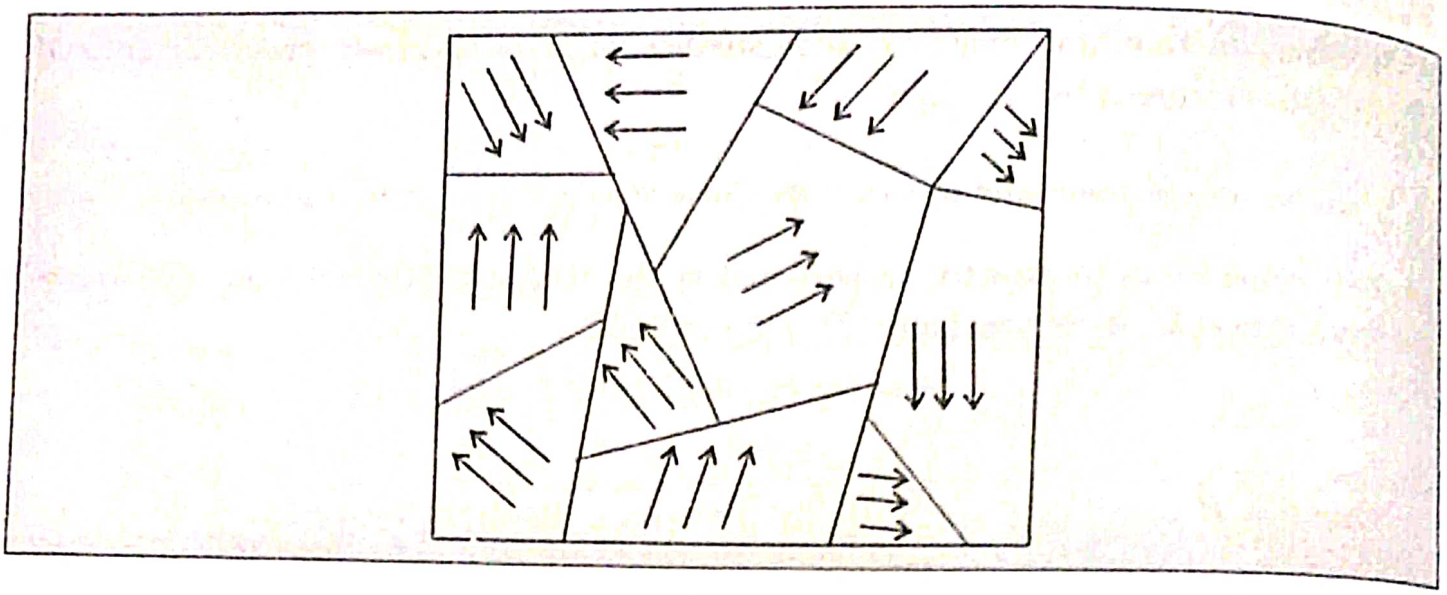


Fig. 3.15

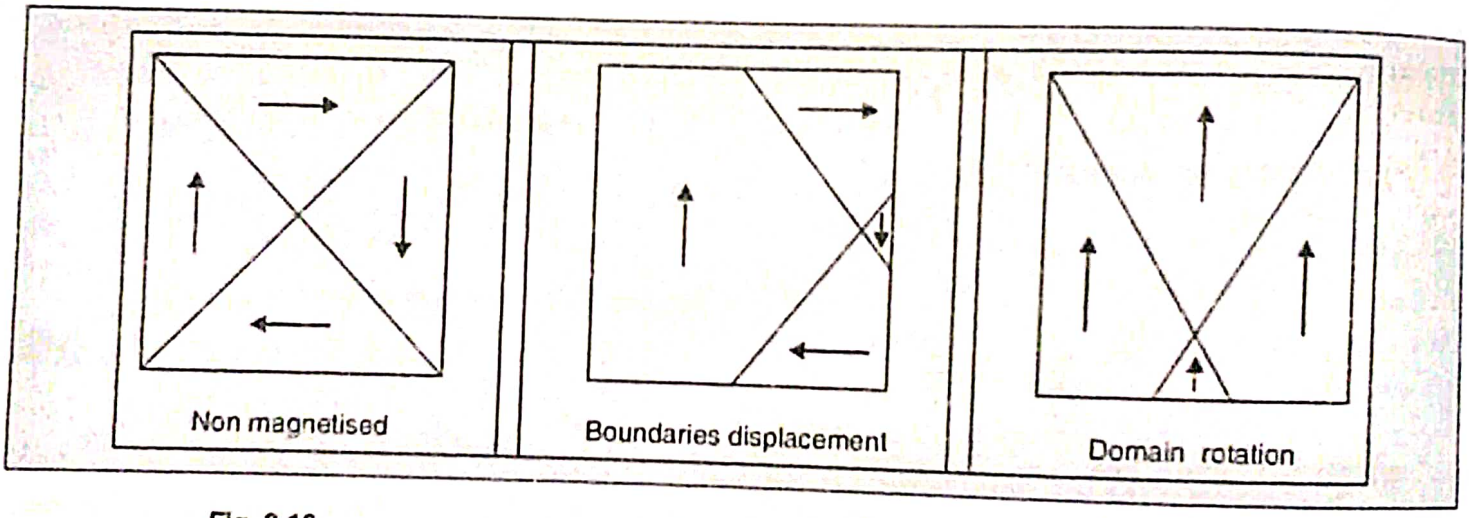


Fig. 3.16 Fig. 3.17 Fig. 3.18

When a ferromagnetic substance is placed in an external magnetic field, the magnetic moment (i.e. magnetism) of the substance increases in different ways.

1. By the Displacement of the Boundaries of the Domain

When an external magnetic field of small strength is applied, then domains pointing approximately in the direction of magnetic field grow at the expense of domains, which are not parallel to applied magnetic field. The magnetization acquired by specimen is small in magnitude. If the strength of applied magnetic field is increased, then magnetization increases due to further growth in size of domains by further displacement of boundaries of the domains having magnetization in direction of applied magnetic field while the size of domain in direction opposite to the external magnetic field decreases as shown in Fig. 3.17. The process continues until all the favourably oriented domains attain maximum volume. At this stage, each domain is still magnetized but all the domains are not in the direction of applied field and magnetization of the sample is still less than the maximum value, it can attain (called saturation magnetization).

2. Rotation of Domains

If strength of applied magnetic field is increased further the magnetic domains which are not in the direction of applied field rotate as a single entity as shown in Fig. 3.18. Ultimately at some value of strength of applied magnetic field, all the domains are oriented in the direction of applied magnetic field. The magnetization of the sample is maximum at this stage and this value is called **saturation** magnetization. With further increase in applied magnetic field (H), magnetization remains constant.

If the external magnetic field is decreased then magnetization of the sample also decreases but not in the same proportion as was during the magnetization of the specimen. Thus domains do not return back to original positions on complete removal of magnetic field. Thus material becomes permanent magnet after the removal of external field.

Evidence in Support of Domain Theory

(i) It is obserbed that when oil with a suspension of fine particles of ferromagnetic material is applied to ferromagnetic substance, then the particles of ferromagnetic powder collects on the domain boundaries as magnetic field is non-uniform there.

(ii) **Magnetostriction.** Magnetostriction is the change in the size of ferromagnetic substance on being subjected to the magnetic field.

3.9 WEISS THEORY OF FERROMAGNETISM

Ferromagnetism arises when the magnetic moments of adjacent atoms are arranged in a regular order i.e. all pointing in the same direction. The ferromagnetic substance thus possess a magnetic moment even in absence of the applied magnetic field. This magnetization is called spontaneous magnetization. It is stable only below a certain critical temperature called Curie temperature. This suggests that electron spins and magnetic moments are arranged in a regular manner. Of the elements only Fe, Ni, Co, Gd and Dy are ferromagnetic although there are some ferromagnetic alloys and oxides also. Above Curie temperatue spontaneous magnetization vanishes and the material becomes paramagnetic.

Weiss theory of magnetism is based on two hypothesis.

(i) The atomic magnets of a ferromagnetic substance are groped into number of certain regions or domains which are spontaneously magnetized.

(ii) Within each domain, the spontaneous magnetization is due to the existence of a molecular field which tends to produce a parallel alignment of the atomic dipoles. This internal field is equivalent to magnetic field Hm which is proportional to the intensity of magnetization I within a domain.

or $$H_m \propto I$$

or $$H_m = \lambda I \qquad \ldots(3.60)$$

Where λ is Weiss constant and is independent of temperature.

If the external magnetic field H is applied, then the effective magnetic field on atomic dipole is equal to

$$H_{eff} = H + \lambda I \qquad \ldots(3.61)$$

Using Langevin's theory of paramagnetism, we have

$$I = N\mu_m L(x) \quad \text{[using eq. (3.53)]} \quad \ldots(3.62)$$

Where N = Number of dipoles per unit volume

μ_m = individual magnetic moment

$L(x)$ = Langevin's function

Here, $N\,\mu_m$ is saturation magnetization (Is) corresponding to situation when all the moments are aligned along the applied magnetic field direction.

i.e. $$Is = N\mu_m \quad \ldots(3.63)$$

Putting this value in eq. (3.62), we get

$$I = Is\, L(x)$$

Where $$L(x) = \left(\coth x - \frac{1}{x}\right)$$

$$\therefore \quad \frac{I}{Is} = L(x) = \left(\coth x - \frac{1}{x}\right) \quad \ldots(3.64)$$

where $$x = \frac{\mu_m B}{kT} \quad \text{[Using eq. (3.49)]}$$

or $$x = \frac{\mu_m \mu_0 H_{eff}}{kT} \quad (\because B = \mu_0 H_{eff}) \quad \ldots(3.65)$$

or $$x = \frac{\mu_m \mu_0 (H + \lambda I)}{kT} \quad \text{using eq. (3.61)}$$

For ferromagnetism, spontaneous magnetization can take place even when $H = 0$.

$$\therefore \quad x = \frac{\mu_m \mu_0 \lambda I}{kT}$$

or $$I = \frac{xkT}{\mu_m \mu_0 \lambda} \quad \ldots(3.66)$$

$$\therefore \quad \frac{I}{Is} = \frac{xkT}{\mu_m \mu_0 \lambda} \times \frac{1}{N\mu_m} \quad \text{using eqs. (3.63 \& 3.66)}$$

or $$\frac{I}{Is} = \frac{xkT}{\mu_0 \lambda N \mu_m^2} \quad \ldots(3.67)$$

In this case, equations (3.64) and (3.67) together determine the condition of spontaneous magnetization. Both these equations can be solved for variables $\frac{I}{Is}$ and x graphically.

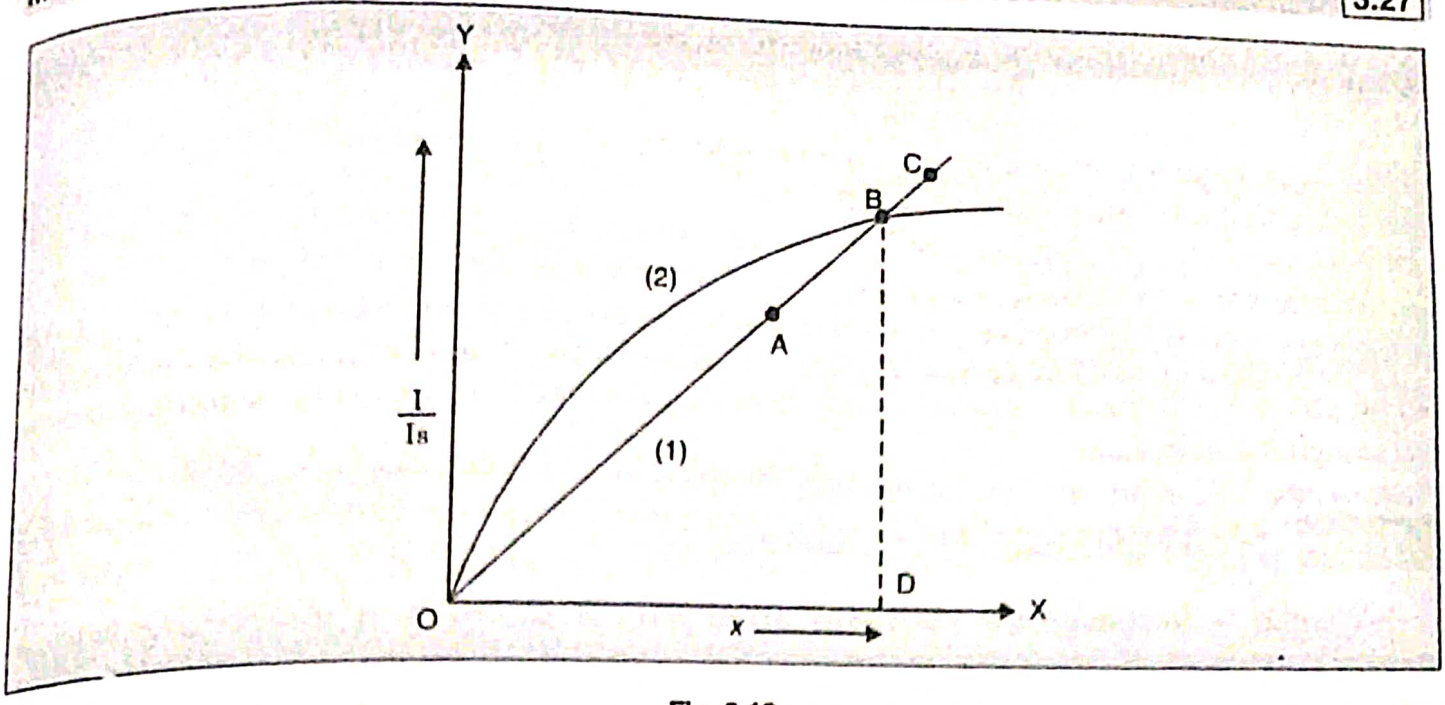


Fig. 3.19

Fig. (3.19) shows the graph between $\frac{I}{Is}$ versus x for equations (3.64) and (3.67). Straight line curve (1) corresponds to equation (3.67) and curve (2) is Langevin curve corresponding to eq. (3.64).

As shown in Fig. 3.19, the two curves meet at O and B.

The solution $\frac{I}{Is} = 0$ is not true, therefore

$$\frac{I}{Is} = BD$$

As shown in Fig. 3.19, B corresponds to stable state of spontaneous magnetization. If the molecules in a domain assumes state A, then the local magnetization is less than the corresponding equilibrium state B. Now, the magnetization and the value of x will in consequence increase until the state BD is reached. On the other hand, if the molecules in a domain assume state C, then the local magnetization is more than the equilibrium state B. Now, the magnetization and the value of x will tend to decrease until the state BD is reached.

The slope of the straight line curve (1) is given as

$$\text{Slope of straight line curve} = \frac{kT}{\mu_0 \lambda N \mu_m^2} \qquad \text{using eq. (3.67)} \quad ...(3.68)$$

For $x \to 0$, then $L(x) = \frac{x}{3}$. So, the slope of straight line is $\frac{1}{3}$.

$\therefore$ Slope of straight line curve becomes

$$\frac{kT}{\mu_0 \lambda N \mu_m^2} = \frac{1}{3}$$

or $$T = \frac{\mu_0 \lambda N \mu_m^2}{3k} \quad \ldots(3.69)$$

or $$T_c = \frac{\mu_0 \lambda N \mu_m^2}{3k} \quad \ldots(3.70)$$

Where $T = T_c$ is Curie temperature.

Hence state of magnetization is possible even without applied field, for temperature below Curie temperature. Above Curie temperature, the ferromagnetic materials become paramagnetic materials.

3.10 HYSTERESIS (B-H CURVE)

Consider a ferromagnetic substance (iron bar) is placed in a magnetizing field. As magnetizing field H is slowly increased, the intensity of magnetization also increases. Fig. (3.20) shows the graphical representation of the extent of magnetization at different values of H. To start with $H = 0$ and magnetization B is also zero. As H increases B also increases along the curve OA. State of saturation is reached at A and further increase of H will not increase B.

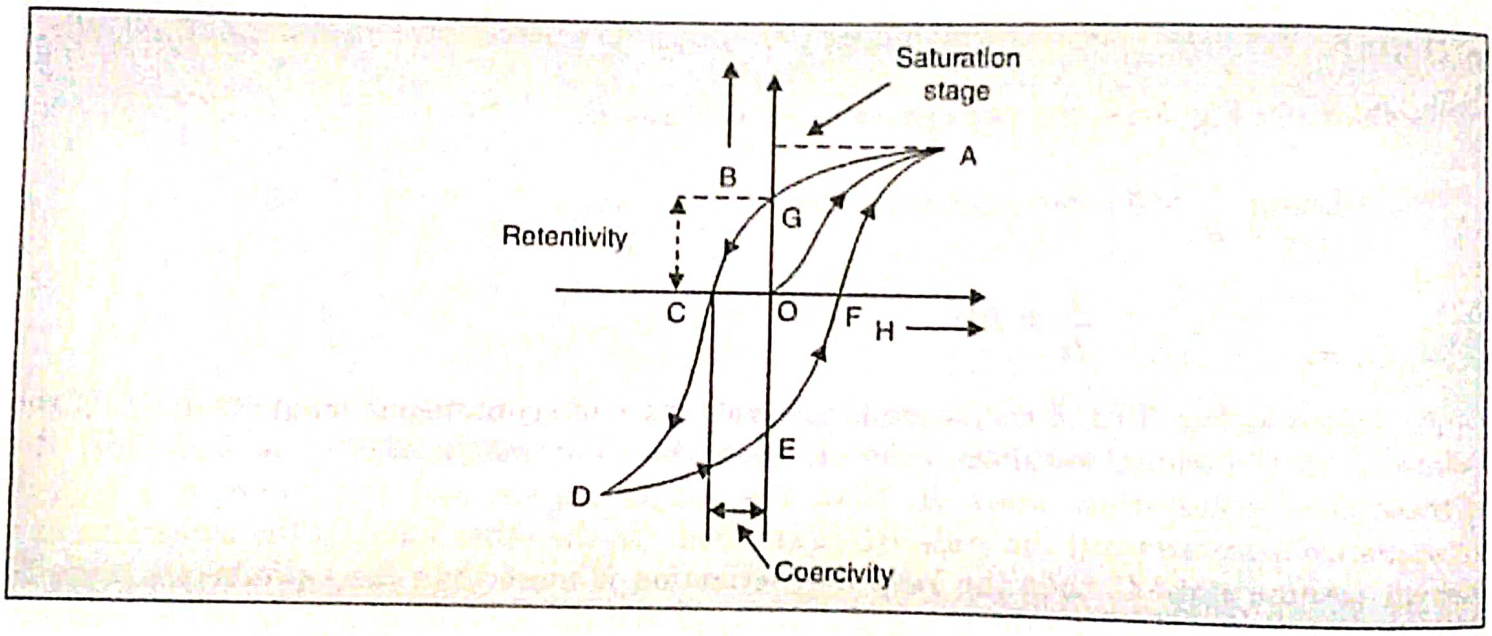


Fig. 3.20

Now if we decrease H, the demagnetization of the sample does not take place along the curve AO. Thus as H is decreased and becomes zero then it is seen that B does not become zero but has the value OG called retentivity. Hence damagnetisation lags behind the magnetizing field H. This phenomena in which B lags behind the magnetizing field H is called Hysteresis. The residual magnetism left behind in the magnetic substance when magnetizing field is reduced to zero is called retentivity. It gives magnetization retained by the sample, when it behaves like a permanent magnet. The value of B at point G is called remanent magnetic induction. Now when H is increased in negative (opposite) direction, B also decreases along GC and at 'C' B reduces to zero. The value of H given by OC is called coercivity.

The magnetizing field (H) in the negative direction required to make B zero is called coercivity.

This gives the ability of the ferromagnetic substance to remain magnetized even when subjected to demangnetising field. Further increase of H in reverse direction magnetise the sample in the opposite direction attaining the saturation state of magnetization at 'D'. The increase of H from this state takes the sample through the path DEFA to the saturated magnetization again in the initial direction. The variation of magnetization represented by AGCDEFA is called **cycle of magnetization.** The closed curve AGCDEFA is called **hysteresis loop.**

Thus lagging of magnetization B behind the magnetizing field H, when the ferromagnetic substance is taken through a complete cycle of magnetization is called hysteresis.

3.11 ENERGY LOSS DUE TO HYSTERESIS

Consider a ferromagnetic sample of unit volume taken through a complete cycle of magnetization.

Let the ferromagnetic sample is having n atomic dipoles per unit volume. Let each dipole has magnetic moment μ_m. At any state of magnetization, let magnetic dipole moment μ_m makes angle θ with the direction of magnetizing field $\vec{H}$ as shown in Fig. (3.21).

The magnetic moment μ_m can be resolved into two components (i) $\mu_m \sin\theta$ perpendicular to $\vec{H}$ and (ii) $\mu_m \cos\theta$ along the direction of $\vec{H}$.

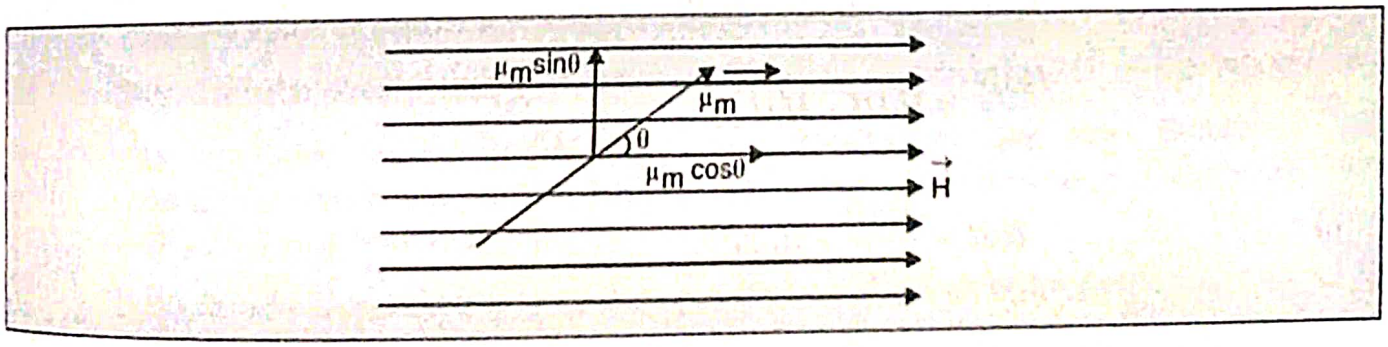


Fig. 3.21

Since there is no magnetization perpendicular to $\vec{H}$, so the sum of all the components of μ_m perpendicular to $\vec{H}$ is zero.

i.e. $\Sigma\mu_m \sin\theta = 0$ (i.e. magnetic moment per unit volume perpendicular to field $\vec{H}$). The magnetic moment per unit volume (i.e. intensity of magnetization I) parallel to field $\vec{H}$.

$$\therefore \quad I = \Sigma\mu_m \cos\theta \qquad \ldots(3.71)$$

when I is increased by an amount dI, then

$$dI = d\Sigma\mu_m \cos\theta = \Sigma\mu_m\, d(\cos\theta)$$

or $$dI = -\Sigma\mu_m \sin\theta\, d\theta \quad \ldots(3.72)$$

The negative sign shows that I decreases at θ increases. Torque acting on magnetic dipole placed in magnetic field $\vec{H}$ is

$$\vec{\tau} = \vec{\mu}_m \times \vec{H}$$

or $$\tau = \mu_m H \sin\theta \quad \ldots(3.73)$$

Work done when dipole rotates through small angle $(-d\theta)$ is given by

$$dW = \tau\,(-d\theta)$$

$$dW = -\mu_m H \sin\theta\, d\theta \quad \text{using eq. (3.73)}$$

$$dW = HdI \quad \ldots(3.74) \text{ using eq. (3.72)}$$

Total work done in taking the substance through a complete cycle of magnetization is

$$W = \oint dW = \oint HdI = \text{Area of } I\text{–}H \text{ loop.}$$

Since $$B = \mu_0\,(H + I)$$

$\therefore$ $$dB = \mu_0\,(dH + dI)$$

Multiplying both the sides by H

$$HdB = \mu_0\,(HdH + HdI)$$

or $$\frac{HdB}{\mu_0} = HdH + HdI$$

or $$HdI = \frac{HdB}{\mu_0} - HdH$$

$$dW = \frac{HdB}{\mu_0} - HdH \quad \text{using eq. (3.74)}$$

$\therefore$ work done during one complete cycle of magnetization is

$$W = \oint dW = \frac{1}{\mu_0}\oint HdB - \oint HdH$$

$$= \frac{1}{\mu_0}\oint HdB - 0$$

$$= \frac{1}{\mu_0}\oint HdB$$

$$\therefore \quad W = \frac{1}{\mu_0} \text{ (area of B-H curve)}$$

Hence energy loss per unit volume during one complete cycle of magnetization is equal to $\frac{1}{\mu_0}$ times the area of B-H loop. This loss of energy appears in the form of heat.

3.12 ANTI FERROMAGNETISM

There are certain materials in which the interacting atoms are very close to each other and exchange forces produce a tendency for antiparallel alignment of electron spins of neighbouring atoms as shown in Fig. (3.22). The resultant magnetic moment for such materials is zero, in the absence of the external magnetic field. But it has a temperature dependent magnetism due to disruption of spin magnetic moment alignment. Such materials are known as antiferromagnetic materials. Examples are copper chloride, oxides of manganese, cobalt and nickel etc.

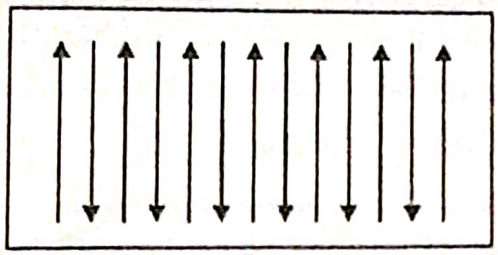


Fig. 3.22

Properties of Antiferromagnetic Materials

1. Electron spins of atoms are aligned antiparallel.
2. The magnetic susceptibility of antiferromagnetic material is very small but positive.
3. The magnetic susceptibility of antiferromagnetic material increases with temperature upto temperature T_N (called Neel temperature) but then decreases with increasing temperature.
4. Below Neel's temperature (T_N), the spin system tends to order in similar way as the spins of a ferromagnetic substances.

   For $T < T_N$

   $\chi \propto T$

   And for $T > T_N$

   $$\chi = \frac{C}{\theta + T}$$

   where C is Curie constant.
5. Antiferromagnetic materials possess dipole moment due to spin of electrons.
6. High magnetic permeability and high electric resistance.

3.13 FERRIMAGNETIC MATERIALS (FERRITES)

Ferrimagnetism is a special case of anti-ferromagnetism. Ferrites are the materials which possess magnetic dipole moment due to spin of electrons and also adjacent atoms are aligned in antiparallel directions. But the magnetic moment of those oriented in one direction is greater than those oriented in opposite direction i.e. spin alignment is antiparallel and of different magnitudes as shown in Fig. (3.23). As a result, there is a net magnetization in the material. These materials are known as Ferrites (or ferrimagnetic materials). Examples : $MnFe_2O_4$, $FeFe_2O_4$ or magnetite, $CoFe_2O_4$, $NiFe_2O_4$, $CuFe_2O_4$ and $MgFe_2O_4$.

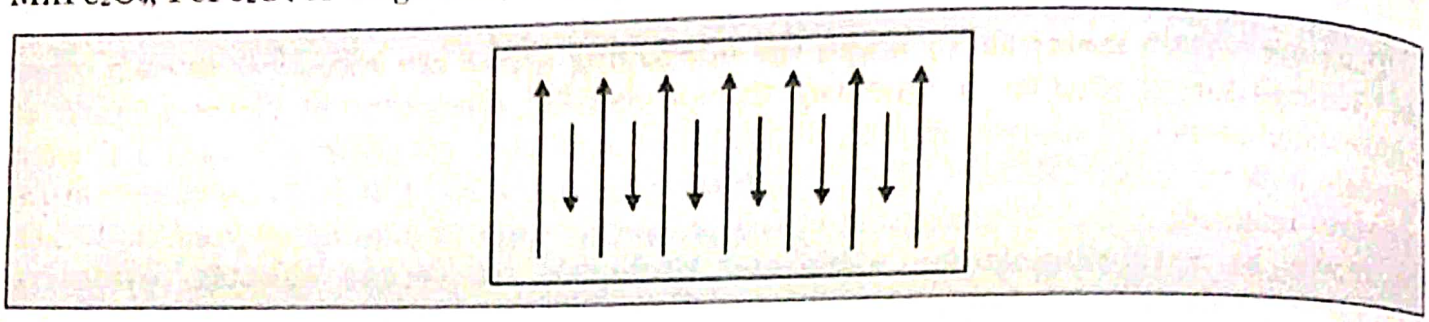


Fig. 3.23

Properties of Ferrites

1. Spin alignment is antiparallel of different magnitudes.
2. Ferrites possess net magnetic moment.
3. All Ferrites fall under a general chemical formula

   $MOFe_2O_3$

   Where, M stands for any divalent ion

   i.e. Co, Ni, Cu, Zn, Cd, etc.
4. Magnetisation of ferrites can be controlled by changing composition.
5. Above Curie temperature ferrites become paramagnetic, below Curie temperature they behave as ferrites.
6. They are electric insulators but possess magnetic properties similar to ferromagnetic materials including hysteresis.
7. The variation of susceptibility with temperature is shown in Fig. 3.24.

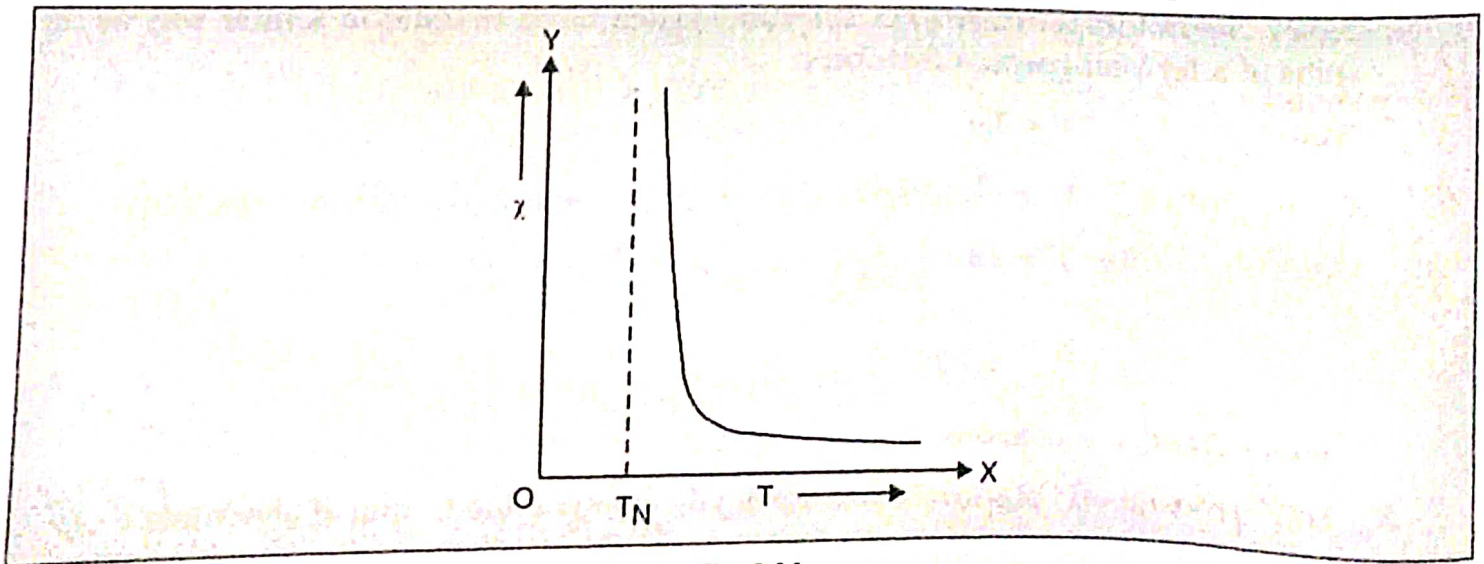


Fig. 3.24

The susceptibility is positive and large $\chi = \frac{C}{T \pm 0}$ for $T > T_N$ Ferrites.

Paramagnetic $T < T_N$.

8. The hysteresis loop of ferrites is nearly rectangular.
9. Ferrites have high permeability.
10. Ferrites have low hysteresis.
11. Ferrites have high resistivity.
12. Because of their poor electrical conductivity, ferrites are used as the cores of devices operating with high frequency currents.

SOLVED PROBLEMS

PROBLEM 1. **A bar magnet of length 10 cm has pole strength of 10 NT^{-1}. Calculate its magnetic dipole moment.**

Solution

Here $2l = 10 \text{ cm} = \frac{10}{100} m = 0.1\ m$

$m = 10\ NT^{-1}$

Magnetic dipole moment $= 2\ ml = m\ (2l)$

$= 10 \times 0.1 = 1\ Am^2$.

PROBLEM 2. **An electron revolves around the nucleus in an orbit of radius 0.54 Å. The frequency of revolution is 6.5×10^{15} Hz. Determine the magnetic moment of electron.**

Solution

Given $r = 0.54\text{Å} = 0.54 \times 10^{-10}\ m = 54 \times 10^{-12}\ m$

$\nu = 6.5 \times 10^{15}$ Hz

Magnetic moment of electron μ_m (or M)

$$\mu_m = IA = I\ (\pi r^2)$$

$$= \frac{e}{T}(\pi r^2) \qquad \left(\because \nu = \frac{1}{T}\right)$$

$$= \pi e \nu r^2$$

$$= 3.14 \times 1.6 \times 10^{-19} \times 6.5 \times 10^{15} \times (54 \times 10^{-12})^2$$

$$= 9.52 \times 10^{-24}\ Am^2$$

PROBLEM 3. Calculate the value of Bohr's magneton. Given $e = 1.6 \times 10^{-19}$ C, $h = 6.64 \times 10^{-34}$ J-s and $m = 9.1 \times 10^{-31}$ kg.

Solution

Given $e = 1.6\times10^{-19} C, h = 6.64\times10^{-34}$ J-s.

$m = 9.1 \times 10^{-31}$ kg.

Bohr's magneton

$$\mu_B = \frac{eh}{4\pi m}$$

$$= \frac{1.6\times10^{-19}\times6.64\times10^{-34}}{4\times3.14\times9.1\times10^{-31}}$$

$$= 9.27 \times 10^{-24}\ J/T \text{ or } Am^2$$

PROBLEM 4. The magnetic induction in a material placed in a magnetizing field of 3000 Am^{-1} is 2 $NA^{-1}\ m^{-1}$. Calculate (i) magnetic permeability (ii) magnetic susceptibility and (iii) intensity of magnetization of the material.

Solution

Given $H = 3000\ Am^{-1}$

$B = 2\ NA^{-1}\ m^{-1}$

(i) $\mu = \frac{B}{H} = \frac{2}{3000} = 0.67\times10^{-3} = 6.7\times10^{-4}\ NA^{-2}$

(ii) $\mu_r = \frac{\mu}{\mu_0} = \frac{6.7\times10^{-4}}{4\pi\times10^{-7}} = \frac{6.7\times10^{3}}{4\times3.14} = \frac{6.7}{12.56}\times10^{3} = 533$

$\therefore \quad \chi_m = \mu_r - 1 = 533 - 1 = 532$

(iii) $\chi_m = \frac{I}{H}$

or $I = \chi_m \times H = 532 \times 3000 = 1.596 \times 10^6\ Am^{-1}$

PROBLEM 5. In a bar of cross-sectional area 0.4 cm^2, a magnetizing field of 1300 Am^{-1} produces a flux density of 1.5 T. Calculate the (i) magnetic flux (ii) permeability and (iii) susceptibility of the bar.

Solution

Given $A = 0.4\ cm^2 = 0.4\times10^{-4}\ m^2 = 4\times10^{-5}\ m^2$

$H = 1300\ Am^{-1}, B = 1.5T$

(i) $\phi = BA = 1.5\times4\times10^{-5} = 6\times10^{-5}\ Wb$

(ii) $\mu = \frac{B}{H} = \frac{1.5}{1300} = 1.15 \times 10^{-3}\ NA^{-2}$

(iii) $\mu_r = \frac{\mu}{\mu_0} = \frac{1.15 \times 10^{-3}}{4\pi \times 10^{-7}} = \frac{1.5}{4 \times 3.14} \times 10^4$

$= \frac{1.5}{12.56} \times 10^4 = 1194.3$

$\chi_m = \mu_r - 1$

$= 1194.3 - 1 = 1193.3$

PROBLEM 6. **The magnetic susceptibility of a medium is 899 × 10^{-11}. Calculate (i) relative permeability and (ii) absolute permeability.**

Solution

Given $\chi_m = 899 \times 10^{-11}$

(i) $\mu_r = 1 + \chi_m = 1 + 899 \times 10^{-11}$

(ii) $\mu_r = \frac{\mu}{\mu_0}$

or $\mu = \mu_r \times \mu_0 = 4\pi \times 10^{-7} \times (1 + 899 \times 10^{-11})\ TmA^{-1}$

PROBLEM 7. **An iron rod of 0.5 cm^2 area of cross section is subjected to a magnetizing field of 1200 Am^{-1}. If susceptibility of iron is 599. Calculate (i) μ (ii) B and (iii) ϕ (magnetic flux produced).**

Solution

Given $A = 0.5\ cm^2 = 0.5 \times 10^{-4}\ m^2$

$H = 1200\ Am^{-1},\ \chi_m = 599$

(i) We know that $\mu_0 = 4\pi \times 10^{-7}\ TA^{-1}m$

$\mu_r = 1 + \chi_m$

$\mu_r = 1 + 599 = 600\ TA^{-1}\ m$

$\mu_r = \frac{\mu}{\mu_0}$

or $\mu = \mu_0 \mu_r = 4\pi \times 10^{-7} \times 600$

$= 4 \times 3.14 \times 10^{-7} \times 600$

$= 7.54 \times 10^{-4}\ TA^{-1}\ m$

(ii) $B = \mu H = 7.54 \times 10^{-4} \times 1200 = 9.05 \times 10^{-1} = 0.905\ T$

(iii) $\phi = BA = 0.905 \times 0.5 \times 10^{-4} = 4.525 \times 10^{-5}\ Wb$

PROBLEM 8. For a magnetizing field of intensity 2×10^3 Am^{-1}, aluminimum at 280 K acquires intensity of magnetization of 4.8×10^{-2} Am^{-1}. Find the subsceptibility of aluminium at 280 K. If the temperature of aluminium is raised to 320 K, what will be the susceptibility and intensity of magnetization ?

Solution

Given $H = 2 \times 10^3\ Am^{-1}$, $T = 280\ K$

$$I = 4.8 \times 10^{-2}\ Am^{-1}$$

$$\chi_m = \frac{I}{H} = \frac{4.8 \times 10^{-2}}{2 \times 10^3} = 2.4 \times 10^{-5}$$

Aluminium is a paramagnetic substance and hence obeys Curie law. If χ'_m is susceptibility of aluminium at 320 K, then,

$$\frac{\chi'_m}{\chi_m} = \frac{T}{T'} \quad \text{or} \quad \chi'_m = \frac{T}{T'} \times \chi_m$$

$$= \frac{280}{320} \times 2.4 \times 10^{-5}$$

$$\therefore \quad \chi'_m = 2.1 \times 10^{-5}$$

If I' is intensity of magnetization of aluminium at 320 K then

$$\chi'_m = \frac{I'}{H}$$

or $$I' = \chi'_m H = 2.1 \times 10^{-5} \times 2 \times 10^3 = 4.2 \times 10^{-2}\ Am^{-1}$$

PROBLEM 9. A sample of paramagnetic salt contains 2.0×20^{24} atomic dipoles, each of dipole moment 1.5×10^{-23} JT^{-1}. The sample is placed under homogeneous magnetic field of 0.84T and cooled to a temperature of 4.2 K. The degree of magnetic saturation achieved is equal to 15%. What is the total dipole moment of the sample for a magnetic field of 0.98 T and a temperature of 2.8 K (assume Curie's law).

Solution

Magnetic dipole moment of each dipole = 1.5×10^{-23} JT^{-1}

Number of atomic dipoles = 2.0×10^{24}

$\therefore$ Total magnetic dipole moment of the sample,

$$M = 1.5 \times 10^{-23} \times 2 \times 10^{24} = 30\ JT^{-1}$$

At temperature of 4.2 K, the magnetic saturation is 15%.

Therefore dipole moment achieved at 4.2 K,

$$M_1 = 30 \times \frac{15}{100} = 4.5 JT^{-1}$$

According to Curie's law

$$M \propto \frac{B}{T}$$

or $$\frac{M_1}{M_2} = \frac{B_1}{T_1} \times \frac{T_2}{B_2}$$

or $$M_2 = M_1 \times \frac{T_1}{T_2} \times \frac{B_2}{B_1}$$

$$= 4.5 \times \frac{4.2}{2.8} \times \frac{0.98}{0.84}$$

[$\because$ $B_1 = 0.84T$ and $B_2 = 0.98T$

$T_1 = 4.2K$, $T_2 = 2.9K$]

$$= \frac{4.5 \times 4.2 \times 0.98}{2.8 \times 0.84}$$

$$= 7.875 JT^{-1}$$

PROBLEM 10. An iron sample of mass 8.4 kg is repeatedly taken over cycles of magnetization and demagnetization at a frequency of 50 cycles per second. It is found that energy equal to 3.2×10^4 J is dissipated as heat in the sample in 30 minutes. If the density of iron is 7200 kg m^{-3}, calculate the value of energy dissipated per unit volume per cycle in the iron sample.

Solution

Let Q be the energy dissipated per unit volume per second in a given iron sample. Then total energy lost by the sample in a given time t

$$W = Q \times V \times \nu \times t$$

where V is volume of the sample and ν is frequency of magnetization and demagnetization.

Here $W = 3.2 \times 10^4$ J, $\nu = 50$ cycles sec^{-1}

$$V = \frac{\text{Mass}}{\text{density}} = \frac{8.4}{7200} \text{ kg m}^{-3}$$

$t = 30$ minutes $= 30 \times 60 = 1800$ second

$\therefore$ $$Q = \frac{W}{V \times \nu \times t} = \frac{3.2 \times 10^4 \times 7200}{8.4 \times 50 \times 1800}$$

$$= 304.8 \text{ Jm}^{-3} \text{ cycle}^{-1}$$

PROBLEM 11. The hysteresis loop of a transformer has 2500 ergs cm^{-3}, calculate the loss of energy per hour at 50 Hz frequency. Density of iron is 7.5 gm cm^{-3} and weight is 10 kg.

Solution

Loss of energy per unit volume per cycle = 2500 ergs cm^{-3}

$\therefore$ Loss of energy per unit volume per hour = $50 \times 60 \times 60 \times 2500$ erg cm^{-3}

$$\text{Volume of iron} = \frac{\text{Mass}}{\text{density}} = \frac{10 \times 1000}{7.5} \text{ kg } m^{-3}$$

$$\therefore \text{ Total loss of energy per hour} = \frac{50 \times 60 \times 60 \times 2500 \times 10 \times 1000}{7.5}$$

$= 6 \times 10^{11}$ Joules

CONCEPTUAL QUESTIONS

Q. 1. What are non-magnetic substances ?

Ans. There are certain atoms in which the electrons are completely paired i.e. for each electron spinning in one direction, there is an electron spinning in the opposite direction. Thus the net current circulating in the atom is zero. The resultant magnetic moment of the atom is zero. Such materials are called non-magnetic substances.

Q. 2. What do you mean by atomic dipole ?

Ans. In an atom, electrons revolve around the nucleus in circular orbits, may be considered as small current loops. Due to this, an atom possesses magnetic dipole moment and hence behave as magnetic dipole.

The magnetic dipole moment of an atom is given as

$$M = \frac{nch}{4\pi m}$$

Q. 3. What is Bohr magneton ? Calculate its value.

Ans. The minimum value of orbital magnetic moment of electron (for n = 1) is called Bohr magneton and it is given as

$$\mu_B = \frac{eh}{4\pi m}$$

The numerical value of Bohr magneton

$$\mu_B = \frac{eh}{4\pi n} = \frac{(1.6 \times 10^{-19} C) \times (6.62 \times 10^{-34} J - s)}{4 \times 3.14 \times (9.1 \times 10^{-31} kg)}$$

$$= 9.27 \times 10^{-24} Am^2$$

Q. 4. How do you classify magnetic substances ?

Ans. Magnetic substances can be classified into three types :

(i) Diamagnetic Substances. These substances are repelled by a magnet. They are magnetized in direction opposite to the applied magnetic field. Examples, Cu, Zn, Ag, Pb etc.

(ii) Paramagnetic Substances. They get magnetized weakly in the direction of applied magnetic field. Examples : Al, Pt, Mn etc.

(iii) Ferromagnetic Substances. They become strongly magnetized when placed in a magnetic field in the direction of applied field. Examples : Ni, Co, Fe etc.

Q. 5. The permeability of a substance is 75×10^{-10}. What type of magnetic substance is it ?

Ans. Paramagnetic substance.

Q. 6. What do you understand by the term magnetization ?

Ans. Magnetisation means the alignment of magnetic dipoles of a magnetic substance under the influence of an external magnetic field. When a magnetic substance is placed in the magnetic field, the atomic dipoles tend to align in the direction of field. This is called magnetization of the given sample.

Q. 7. Does the magnetization of a paramagnetic salt depend on temperature ? Give reason for your answer.

Ans. Yes, the magnetization of a paramagnetic salt decreases with increase of temperature. This is because the tendency to disrupt the alignment of atomic dipoles arising from the random thermal motion increases with the increase of temperature.

Q. 8. Why do the magnetic lines of force prefer to pass through a ferromagnetic substance than through air ?

Ans. This is because the magnetic permeability of a ferromagnetic substance is very high.

Q. 9. Why soft iron preferred in electromagnets and transformers ?

Ans. Soft iron is preferred in electromagnets and transformer cores because it has (i) high permeability and (ii) low hysteresis loss.

Q. 10. Why do we use steel or alnico for making permanent magnets ?

Ans. Steel and alnico have high coercivity which is essential for permanent stay of magnetism in the sample. Under rough conditions, the magnetism is not easily lost.

Q. 11. How can a magnet be demagnetized completely?

Ans. A magnet is demagnetized completely if the atomic dipoles are randomly oriented. The alignment of dipoles is broken when their thermal energy increases. Thus, a magnet can be demagnetized completely by heating it.

Q. 12. Why is ferromagnetism not found in liquids and gases ?

Ans. This is because in liquids and gases, complete alignment of atomic dipoles is not possible.

Q. 13. What is gyromagnetic orbital ratio ?

Ans. The ratio of orbital magnetic moment to the angular momentum of the orbiting electron is a number $\left(\frac{e}{2m_e}\right)$ which is independent of the size or shape of the orbit. This ratio is called gyromagnetic orbital ratio.

Q. 14. Why is magnetic susceptibility of diamagnetic substance negative ?

Ans. For diamagnetic substances the intensity of magnetization (I) is opposite to the magnetizing field (H).

Since $\chi_m = \frac{I}{H}$, so magnetic susceptibility of diamagnetic substance is negative.

Q. 15. Define Curie temperature.

Ans. The temperature at which ferromagnetic substance becomes paramagnetic substance.

Q. 16. What do you understand by hysteresis ?

Ans. The lagging of magnetization B behind the magnetizing field H, when the ferromagnetic substance is taken through a complete cycle of magnetization is called hysteresis.

Q. 17. Give some properties of ferrites.

Ans. Ferrites have high permeability, high resistivity, low conductivity and hysteresis loop of rectangular shapes.

Q. 18. What kind of ferromagnetic material is used for coating magnetic tapes in a cassette player or for building memory stores' in a modern computer ?

Ans. Ceramics (specially treated with barium iron oxides also called ferrites).

Q. 19. What is Curie's law ?

Ans. According to this law, magnetic susceptibility (χ_m) is inversely proportional to the absolute temperature of the material.

$$\chi_m \propto \frac{I}{T}$$

Q. 20. What is meant by domains ?

Ans. In ferromagnetic substances, the magnetic moments of individual atoms are coupled to the neighbouring magnetic moments very strongly through exchange interactions. The large number of magnetic dipoles get aligned in the same direction and form large small effective regions called domains.

Q. 21. Write the expression for magnetic susceptibility of a paramagnetic material using "Langevin theory of paramagnetism". Show that it leads to Curie's law.

Ans. The magnetic susceptibility of a paramagnetic material on the bases of 'Langevin theory' is given as

$$\chi_m = \frac{N\mu_0\mu_m^2}{3kT}$$

or $\chi_m = \frac{C'}{T}$ where $C' = \frac{N\mu_0\mu_m^2}{3k}$ is called Curie's constant

or $\chi_m \propto \frac{I}{T}$

This equation shows that magnetic susceptibility of a paramagnetic material is positive and varies inversely as absolute temperature. This is Curie's law.

MULTIPLE CHOICE QUESTIONS

1. **The magnetic moment of a material is zero. The material :**
   (a) must be paramagnetic
   (b) must be ferromagnetic
   (c) must be diamagnetic
   (d) may be paramagnetic or diamagnetic

2. **The strongest diamagnetic material is :**
   (a) bismuth
   (b) hydrogen
   (c) helium
   (d) neon

3. **If a magnetic induction B passes normally through a closed coil of cross sectional area A, then flux ϕ can be expressed as :**
   (a) $\phi = BA^2$
   (b) $\phi = BA$
   (c) $\phi = \frac{B}{A}$
   (d) $\phi = B^2$

4. **Tesla is the S.I. unit of :**
   (a) magnetic flux
   (b) magnetic flux density
   (c) magnetic susceptibility
   (d) Intensity of magnetisation

5. **The unit of magnetic induction is :**
   (a) Weber
   (b) Weber/m^2
   (c) Weber/ampere hr.
   (d) Weber amp./m^2

6. **A magnetic dipole placed in a uniform magnetic field experiences :**
   (a) both a force and a torque
   (b) a force but no torque
   (c) a torque but no force
   (d) neither a force nor a toque

7. **The magnetic moment per unit volume is called**
   (a) magnetic induction
   (b) magnetic permeability
   (c) magnetic susceptibility
   (d) intensity of magnetisation

8. **The temperature at which a ferromagnetic matieral changes into paramagnetic material is known as :**
   (a) critical temperature
   (b) temperature of inversion
   (c) Debye temperature
   (d) Curie's temperature

9. **Which of the following magnetic substances can have positive permeability and negative susceptibility ?**

(a) Ferromagnetic
(b) Paramagnetic
(c) Diamagnetic
(d) None

10. The susceptibility of a diamagnetic material is

(a) Very large
(b) small but positive
(c) small but negative
(d) zero

11. Which of the following has low value for ferrite ?

(a) Conductivity
(b) Permeability
(c) Magnetic susceptibility
(d) None of the above

12. Paramagnetic susceptibility varies as

(a) T
(b) T^2
(c) $\frac{1}{T^2}$
(d) $\frac{1}{T}$

13. The susceptibility of a diamagnetic material is expressed as :

(a) $\frac{-n Ze^2 r_0^2 \mu_m}{6m}$
(b) $\frac{n Ze^2 r_0^2 \mu_m}{6m}$
(c) $\frac{n^2 Ze^2 r_0^2 \mu_m}{6m}$
(d) $\frac{n Z^2 e^2 r_0^2 \mu_m}{6m}$

14. Curie-Weiss law is :

(a) $\chi_m = \frac{C}{T}$
(b) $\chi_m = \frac{C}{\theta}$
(c) $\chi_m = \frac{C}{T-\theta}$
(d) $\chi_m = \frac{T-\theta}{C}$

15. Permanent dipole moment consists of the following angular momentum:

(a) orbital angular momentum of electron
(b) spin angular momentum of electron
(c) Nuclear spin angular momentum
(d) all the above

16. The area of hysteresis loop of ferromagnetic material gives :

(a) the coercive force
(b) remnant flux density
(c) the energy that is consumed in taking the material through a complete cycle of magnetization
(d) the intensity of magnetization of the material

17. The magnetization retained by the specimen when the magnetizing field reduced from saturation value to zero is known as :

(a) coercivity
(b) hysteresis
(c) retentivity
(d) spontaneous magnetisation

18. **Which of the following is diamagnetic ?**
(a) Water (b) Air
(c) Copper sulphate (d) Liquid Oxygen

19. **Magnetic permeability is highest for :**
(a) paramagnetic substances (b) diamagnetic substances
(c) ferromagnetic susbstances (d) vacuum.

20. **The relation between magnetic susceptibility and relative permeability is :**
(a) $\chi = 1 - \mu_r$ (b) $\chi = 1 + \mu_r$
(c) $\mu_r = 1 - \chi$ (d) $\mu_r = 1 + \chi$

21. **The relative permeability of air is :**
(a) 1 (b) 1.3
(c) 0.5 (d) 2

22. **The lagging of magnetic induction behind the magnetizing field is known as :**
(a) hysteresis (b) retentivity
(c) coercivity (d) magnetostriction

23. **The most suitable material for making permanent magnet is :**
(a) nickel (b) copper
(c) steel (d) soft iron

24. **Ferrites are :**
(a) conducting materials of square shaped hysteresis loop.
(b) conducting materials of small area hysteresis loop.
(c) semiconductors of square shaped hystersis loop.
(d) semiconductors of small area hysteresis loop.

Answers

1.	(d)	2.	(a)	3.	(b)	4.	(b)	5.	(b)
6.	(c)	7.	(d)	8.	(d)	9.	(c)	10	(c)
11.	(a)	12.	(d)	13.	(a)	14.	(c)	15.	(d)
16.	(c)	17.	(c)	18.	(b)	19.	(c)	20.	(d)
21.	(a)	22.	(a)	23.	(c)	24.	(c)		

CHAPTER AT A GLANCE

1. Some Important Terms

(i) Magnetic Intensity

$$I = \frac{B_0}{\mu_0}$$

Where B_0 = Magnetic field in a vacuum. $\mu_0 = 4\pi \times 10^{-7}\ TmA^{-1}$ is absolute permeability of vacuum.

(ii) Intensity of Magnetization. It is defined as magnetic moment developed per unit volume, when a magnetic material specimen is placed in a magnetizing field

$$I = \frac{magnetic\,moment}{volume} = \frac{M}{V}\ Am^{-1}$$

Also $I = \frac{m}{a}$ = Pole strength developed per unit area of the specific material

(iii) Magnetic Flux (ϕ). It is defined as number of magnetic lines of force passing normally through a surface.

$$\phi = \vec{B}.d\vec{S}\ \text{Weber (or Wb)}$$

(iv) Magnetic Induction (B). It is defined as number of magnetic lines of induction crossing per unit area normally through a magnetic material.

$$B = \mu_0 (H + I)$$

S.I. units of B are tesla (T)

$$\text{Tesla} = 10^4 \text{ gauss}$$

(v) Magnetic Susceptibility. It is defined as the ratio of intensity of magnetization to the magnetic intensity.

$$\chi_m = \frac{I}{H}$$

It has no units.

(vi) Magnetic Permeability. It is defined as ratio of magnetic induction to the magnetic intensity.

$$\mu = \frac{B}{H}$$

$$\mu_r = 1 + \chi_m$$

where $\mu_r = \frac{\mu}{\mu_0}$ is relative permeability of magnetic substance

2. Atom as a Magnetic Dipole

In atom, electrons revolve around the nucleus in circular orbits, may be considered as small current loops. Due to this, an atom possesses magnetic dipole moment and hence behave as magnetic dipole.

The magnetic dipole moment of the atom is given as :

$$M = n\left(\frac{eh}{4\pi m}\right) = \frac{ne\hbar}{2m} \text{ where } \hbar = \frac{h}{2\pi}$$

Bohr magneton $\mu_B = \frac{eh}{4\pi m} = 9.27 \times 10^{-24}\ Am^2$

3. Magnetic Materials

(i) Diamagnetic Materials. Those materials which when placed in a magnetic field become feebly (weakly) magnetized in a direction opposite to that of applied external magnetic field are called diamagnetic materials.

Examples. Bismuth, antimony, gold, mercury, lead, quartz etc.

(ii) Paramagnetic Materials. The materials which when placed in a magnetic field, becomes feebly (weakly) magnetized, in the direction of applied magnetic field, are called paramagnetic materials.

Examples. Platinum, aluminium, chromium, manganese etc.

(iii) Ferromagnetic Materials. Those materials, which when placed in a magnetic field are strongly magnetized in the direction of the applied magnetic field are called ferromagnetic materials.

Examples. Iron, nickel, cobalt, gadolinium and other alloys.

4. The diamagnetic susceptibility according to classical Langevin's Theory of diamagnetism is given as :

$$\chi_m = \frac{-nZ\mu_0 e^2}{6m}\Sigma r^2$$

5. Langevin's theory of paramagnetism leads to the expression of the susceptibility of paramagnetism

$$\chi_m = \frac{N\mu_0\mu_m^2}{3kT}$$

or $$\chi_m = \frac{C'}{T} \text{ where } C' = \frac{N\mu_0\mu_m^2}{3k} \text{ called Curie's constant}$$

which is Curie's law.

6. **Curie's Law.** According to this law, magnetic susceptibility is inversely proportional to the absolute temperature of the material

$$\chi_m \propto \frac{1}{T}$$

7. **Curie Temperature.** The temperature at which a ferromagnetic substance becomes paramagnetic substance is known as Curie temperature.

8. **Domain Theory of Ferromagnetism.** In case of ferromagnetic substances the magnetic moments of individual atoms are coupled to the neighbouring magnetic moments very strongly through exchange interactions. The large number of magnetic dipoles get aligned in the same direction form large number of small effective regions called domains. However in normal state of substance (when external magnetic field is absent) the different domains are randomly oriented. Hence their resultant magnetic moment is zero. When a

ferromagnetic substance is placed in an external magnetic field, the magnetic moment of the substance increases in two different ways.

(i) By displacement of boundaries of the domain and (ii) Rotation of domains.

9. Weiss Theory of ferromagnetism is based on two hypothesis :

(i) The atomic magnets of a ferromagnetic substance are grouped into number of certain regions or domains which are spontaneously magnetized.

(ii) Within each domain, the spontaneous magnetism is due to existence of a molecular field which tends to produce a parallel alignment of atomic dipoles.

10. Hysteresis is the property of lagging of magnetization behind the magnetic field of ferromagnetic materials.

11. The loss of energy in taking a ferromagnetic material through a complete cycle of magnetization is called hysteresis loss.

12. Anti-Ferromagnetism. There are certain materials in which the interacting atoms are very close to each other and exchange forces produce a tendency for antiparallel alignment of electron spins of neighbouring atoms. The resultant magnetic moment for such materials is zero, in the absence of external magnetic field. But it has a temperature dependent magnetism due to disruption of spin magnetic moment alignment. Such materials are called antiferromagnetic materials.

Examples. Copper chloride, oxides of manganese.

13. Ferrimagnetic Materials (Ferrites)

Ferrimagnetism is a special case of anti-ferromagnetism. Ferrites are the materials which possess magnetic dipole moment due to spin of electrons and also adjacent atoms are aligned in antiparallel directions. But the magnetic moments of those oriented in one direction is greater than those oriented in opposite direction. As a result, there is net magnetization in the material. These materials are known as ferrites.

Examples. Mn Fe_2O_4, $FeFe_2O_4$ or magnetite, $CoFe_2O_4$, $NiFe_2O_4$ etc.

SHORT ANSWER QUESTIONS

1. Define magnetic susceptibility and permeability.
2. What do you understand by the term magnetization ?
3. Distinguish between para, dia and ferromagnetic materials.
4. Explain the classification of magnetic materials.
5. Prove that the magnetic moment due to orbital motion of an electron is equal to integral multiple of $\frac{eh}{4\pi m}$.
6. What are domains ?
7. Discuss domain theory of ferromagnetism.
8. What is Weiss theory of ferromagnetic materials ?

9. What is Curie Law ?
10. What is Curie temperature ?
11. What is hysteresis curve ?
12. What is hyteresis loss ?
13. Write short notes on :
    (i) Classification of magnetic materials.
    (ii) Weiss theory of ferromagnetism.
14. Calculate magnetic moment of an atomic dipole.
15. Explain Langevin's theory of paramagnetism.
16. Explain Langevin's theory of diamagnetism.
17. Define magnetic susceptibility and permeability.
    Prove that $\mu_r = 1 + \chi_m$
18. What are ferrites ?
19. Discuss energy loss from B-H curve.
20. Explain the use of hysteresis curve.

LONG ANSWER QUESTIONS

1. Define intensity of magnetization, magnetic susceptibility and magnetic induction. Prove that
    (i) $B = \mu_0 (H + I)$ and (ii) $\mu_r = (1 + \chi_m)$
2. Distinguish between para, ferro and diamagnetic substances on the basis of their propreties.
3. What are para, ferro and diamagnetic substances ? Give their properties.
4. (i) Prove that magnetic moment due to orbital motion of electron is equal to $\frac{nh}{4\pi m}$
    (ii) Define Bohr magneton ? Give its numerical value.
5. Explain Atomic Theory of Magnetism (Qualitative).
6. Discuss Langevin's theory of Diamagnetism and obtain the expression for diamagnetic susceptibility.
7. Disucss Langevin's theory of paramagnetism and derive and expression for paramagnetic susceptibility.
8. Discuss Domain theory of Ferromagnetism.
9. Explain diagmanetism, paramagnetism and ferromagnetism on the basis of dipoles of atoms.

10. Discuss the Weiss theory of ferromagnetism. Show from Langevin function that ferromagnets lose their spontaneous magnetization above Curie temperature.
11. Explain Curie law and Curie temperature.
12. Give Weiss of Ferromagnetism.
13. Give an expression for paramagnetic susceptibility. How does the paramagnetic susceptibility of a material vary with temperature?
14. Draw the B-H curve for a ferromagnetic material and identify the retentivity and coercivity on the curve.
15. Explain ferromagnetism on the basis of Domain theory.
16. Explain the use of hysteresis curve.
17. Explain what do you understand by Hysteresis, Retentivity and coercivity. How will you determine the value of retentivity and coercivity from a loop ?
18. State Curie's law. What is Curie temperature?
19. Explain the term hysteresis and prove that hysteresis loss per cycle of magnetization is equal to the area of the B-H loop.
20. Write notes :
    (i) Electron spin and paramagnetism.
    (ii) Domain theory of ferromagnetism.
    (iii) Ferrites.
    (iv) Diamagnetism
21. What do you meant by :
    (i) Hysteresis loop and (ii) Ferrites
22. What are ferrites ? How do they differ from ferromagnetic substances ?

UNSOLVED NUMERICAL PROBLEMS

1. The permeability of a magnetic material is measured to be 0.12 TA^{-1}. Find its relative permeability and susceptibility. [Ans. 9.55×10^4, 9.55×10^4]

[Hints. $\mu_r = \frac{\mu}{\mu_0} = \frac{0.12}{4\pi \times 10^{-7}} = 9.55 \times 10^4, \chi_m = \mu_r - 1 = 9.55 \times 10^4 - 1 = 9.55 \times 10^4$]

2. A magnet weighs 75 gm and magnetic moment is 2×10^{-4} Am^2. If the density of material of the magnet is 7.5×10^3 kg m^{-3}, calculate the intensity of magnetization.

[Ans. 20 Am^{-1}]

[Hints. $V = \frac{\text{mass}}{\text{density}} = \frac{75 \times 10^{-3}}{7.5 \times 10^3} = 10^{-5} m^3$, $I = \frac{M}{V} = \frac{2 \times 10^{-4}}{10^{-5}} = 20\ Am^{-1}$]

3. The magnetic induction and magnetizing field in a sample of a magnetic material are 1.0 Wb m^{-2} and 2×10^3 Am^{-1} respectively. Find (a) magnetic permeability (b) relative permeability of the material (c) Magnetic susceptibility and (d) intensity of magnetization. Given $\mu_0 = 4\pi \times 10^{-7}\ TA^{-1}m$.

[Ans. (a) $5 \times 10^{-4}\ TmA^{-1}$ (b) 397.9 (c) 396.9 (d) $7.94 \times 10^5\ Am^{-1}$]

[Hints. $\mu = \frac{B}{H} = \frac{10}{2 \times 10^3} = 5 \times 10^{-4}\ TmA^{-1}$, $\mu_r = \frac{\mu}{\mu_0} = \frac{5 \times 10^{-4}}{4\pi \times 10^{-7}} = 397.9$, $\chi_m = \mu_r - 1$ $= 397.9 - 1 = 396.9$, $I = \chi_m H = 396.9 \times 2 \times 10^3 = 7.94 \times 10^5\ Am^{-1}$]

4. The magnetizing field of 1600 Am^{-1} produces a magnetic flux of 2.4×10^{-5} Weber in a bar of iron of cross-section 0.2 cm^2. Calculate the relative permeability, intensity of magnetization and susceptibility of the bar. [Ans. 596.8, $9.534 \times 10^5\ Am^{-1}$, 595.8]

[Hints. $B = \frac{\phi}{A} = \frac{2.4 \times 10^{-5}}{0.2 \times 10^4} = 1.2T$, $\mu = \frac{B}{H} = \frac{1.2}{1600} = 7.5 \times 10^{-4}\ TmA^{-1}$, $\mu_r = \frac{\mu}{\mu_0}$ $= \frac{7.5 \times 10^{-4}}{4\pi \times 10^{-7}}$ 596.8, $\chi_m = \mu_r - 1 = 596.8 - 1 = 598.8$, $I = \chi_m H = 595.8 \times 1600$ $= 9.534 \times 10^5\ Am^{-1}$]

5. The magnetic susceptibility χ_m of platinum is 30×10^{-5} calculate its absolute permeability and relative permeability. [Ans. 12.57×10^{-7} Wb $A^{-1}\ m^{-1}$, 1.003]

[Hints. $\mu_r = 1 + \chi_m = 1 + 30 \times 10^{-5} = 1.0003$, $\mu = \mu_0 \mu_r = 4\pi \times 10^{-7} \times 1.0003 = 12.57 \times 10^{-7}$ Wb $A^{-1}m^{-1}$]

6. Hystersis loss per cubic meter for soft iron is 10^3 Joules. Taking the density 7.5 gm per cm^3 and specific heat 100 cal $kg^{-1}\ C^{-1}$, calculate the rise of temperature per minute when the specimen is subjected to an alternating magnetic field of frequency 50 cycles/sec. [Ans. $\theta = 0.95°C$]

[Hints. Energy lost per minute per $m^3 = 10^3 \times 50 \times 60$ Joules. Heat generated per minute $= \frac{10^3 \times 50 \times 60}{4.2}$ Cals.

$\frac{\text{Mass of iron}}{cm^3} = 7.5$ gm, Mass of iron per m^3 in kg $= \frac{7.5 \times 10^6}{10^3} = 7.5 \times 10^3$, If θ is rise in temperature.

$7.5 \times 10^3 \times 100 \times \theta = \frac{10^3 \times 50 \times 60}{4.2}$ or $\theta = 0.95°C$]

7. A magnetic field of 2×10^3 mks units produces a flux of 3×10^{-5} Wb in a bar of iron of cross section 0.2 cm^2. Derive the permeability and susceptibility of the specimen.

[Ans. 7.5×10^{-4}, 596]

[Hints. $B = \frac{\phi}{A} = \frac{3\times10^{-5}}{2\times10^{-5}} = 1.5 Wb/m^2, \mu = \frac{B}{H} = \frac{1.5}{2\times10^{3}} = 7.5\times10^{-4}$ $\mu_r = \frac{\mu}{\mu_0} = \frac{7.5\times10^{-4}}{4\pi\times10^{-7}}$

$= \frac{7.5\times10^{-4}}{4\times3.14\times10^{-7}} = 597,\ \chi_m = \mu_r - 1 = 597 - 1 = 596$]

8. The susceptibility of magnesium is 1.2×10^{-5} at room temperature (300 K). Find the susceptibility at 400 K. [Ans. 9×10^{-6}]

[Hints. $\frac{\chi_2}{\chi_1} = \frac{T_1}{T_2}$ or $\chi_2 = \chi_1\left(\frac{T_1}{T_2}\right) = 1.2\times10^{-5}\times\left(\frac{300}{400}\right) = 9\times10^{-6}$]

9. The volume of the core of a transformer is 1000 cm^3. It is fed with A.C of 50 Hz. If the loss of energy due to hysteresis per hour is 36 Joules, calculate the area of B-H loop. [Ans. $0.2\ Jm^{-3}$]

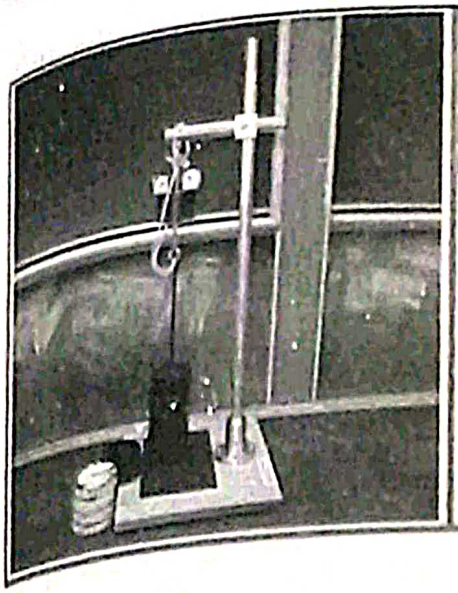
[Hints. Loss of energy/Sec. $= \frac{36}{60\times60} = 10^{-2}$ J/s

Loss of energy per cycle $= \frac{10^{-2}}{50} = 2\times10^{-4}$ J/s/Cycle

Volume of transformer core = 1000 cm^3 = $1000/10^6 = 10^{-3}\ m^3$

Energy loss per cycle per unit volume $= \frac{2\times10^{-4}}{10^{-3}} = 0.2 Jm^{-3}$ = Area of B-H loop]

□□□



Chapter 4

DIELECTRIC PROPERTIES OF MATERIALS

4.1 DIELECTRICS

Dielectrics are the material (insulators) in which all the electrons are tightly bound to the nuclei of atoms. There are no free electrons to carry current. Hence the electrical conductivity of a dielectric is very low. The electrical conductivity of an ideal dielectric is zero. When a dielectric is placed in an external electric field induced charges are produced on its outer surface. Examples of dielectric are glass, mica, wax, air, water etc.

Dielectric Constant

When a dielectric material is introduced between the plates of a capacitor, its capacitance increases. The ratio of the capacitance of a capacitor with a dielectric in between the plates to the capacitance of the same capacitor in vacuum (without dielectric) is called dielectric constant of the material.

If the capacitance of capacitor with dielectric between the plates of the capacitor = C.

Capacitance of the capacitor in vacuum (without dielectric) = C_0

Then dielectric constant of material between the plates of the capacitor.

$$K = \frac{C}{C_0} \qquad \ldots(4.1)$$

It is numerically equal to relative permitivity ϵ_r in S.I. units i.e. $K = \epsilon_r$

Dielectric constant of air or vacuum is equal to one.

4.2 CLASSIFICATION OF DIELECTRICS

In a molecule positive and negative charges are present in equal amounts. The negative charge in the form of electrons cloud are distributed around nuclei having equal positive charges. In such molecules, the centers of gravity of positive and negative charges may or may not coincide. Likewise the molecules are known as non-polar or polar. Thus dielectrics can be divided into two types.

(i) Polar Dielectrics and (ii) Non-Polar Dielectrics

(I) Polar Dielectrics

The dielectrics whose each molecule possesses permanent electric dipole moment are called polar dielectrics. In these molecules the centres of gravity of positive and negative charges do not coincide. These molecules have unsymmetrical shapes. Examples of polar molecules are HCl, NH_3, CO_2, H_2O etc.

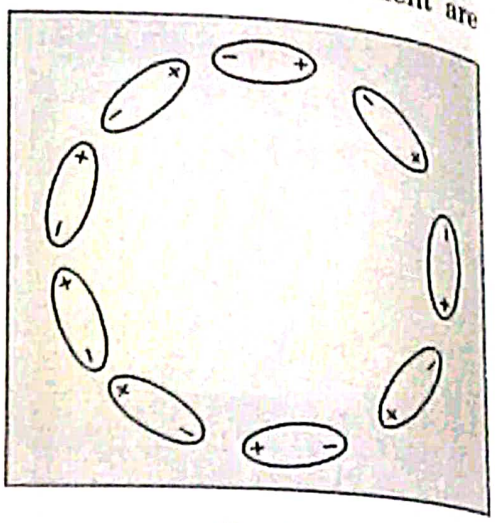


Fig. 4.1

In the absence of external electric field, these polar molecules form closed chains. Hence the net electric dipole moment of these molecules is zero as shown in Fig. (4.1). When an external electric field is applied, these polar molecules experience toque and closed chains are broken and the molecules try to align themselves in the direction of electric field. But this tendency of molecules to align in the direction of electric field is opposed by thermal agitation. The degree of alignment increases with increase of strength of electric field and decrease of temperature.

(ii) Non-Polar Dielectrics

The dielectric is said to be non polar if dipole moment of each molecule of the sample is zero when no external electric field is applied. In these molecules the centres of gravity of positive and negative charges coincides. These molecules have symmetrical shapes. Examples of non polar molecules are H_2, O_2, N_2, Cl_2 etc. In the absence of electric field each molecule has no electric dipole moment as shown in Fig. (4.2). When electric field is applied, all the positive charges in a molecule experience force in the direction of electric field. All the negative charges (electrons) experience force in direction opposite to the direction of electric field. Hence centres of gravity of the positive and negative charges are displaced in opposite directions. Thus each non-polar molecule, in the electric field becomes an induced electric dipole and has induced electric dipole moment as shown in Fig. (4.3).

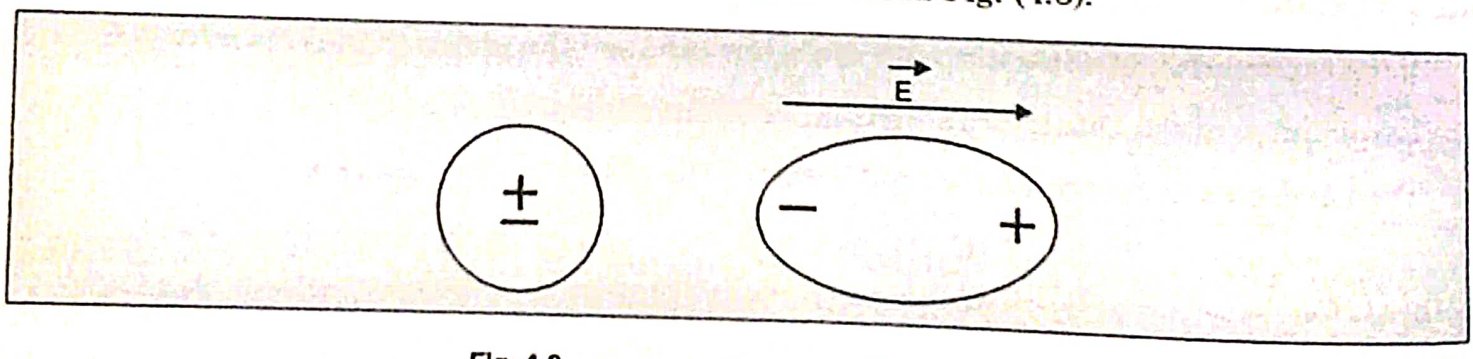


Fig. 4.2 Fig. 4.3

The net effect of external electric field is the same on a dielectric, whether it is polar or non-polar. The molecules get align in the direction of electric field or a dielectric gets polarized.

4.3 POLARIZATION OF DIELECTRIC

If the molecules of a dielectric are polar, then in the absence of external electric field, the molecules are randomly oriented and net dipole moment of the dielectric is zero. In case of dielectric with non-polar molecules, the net dipole of dielectric is zero in the absence of electric field.

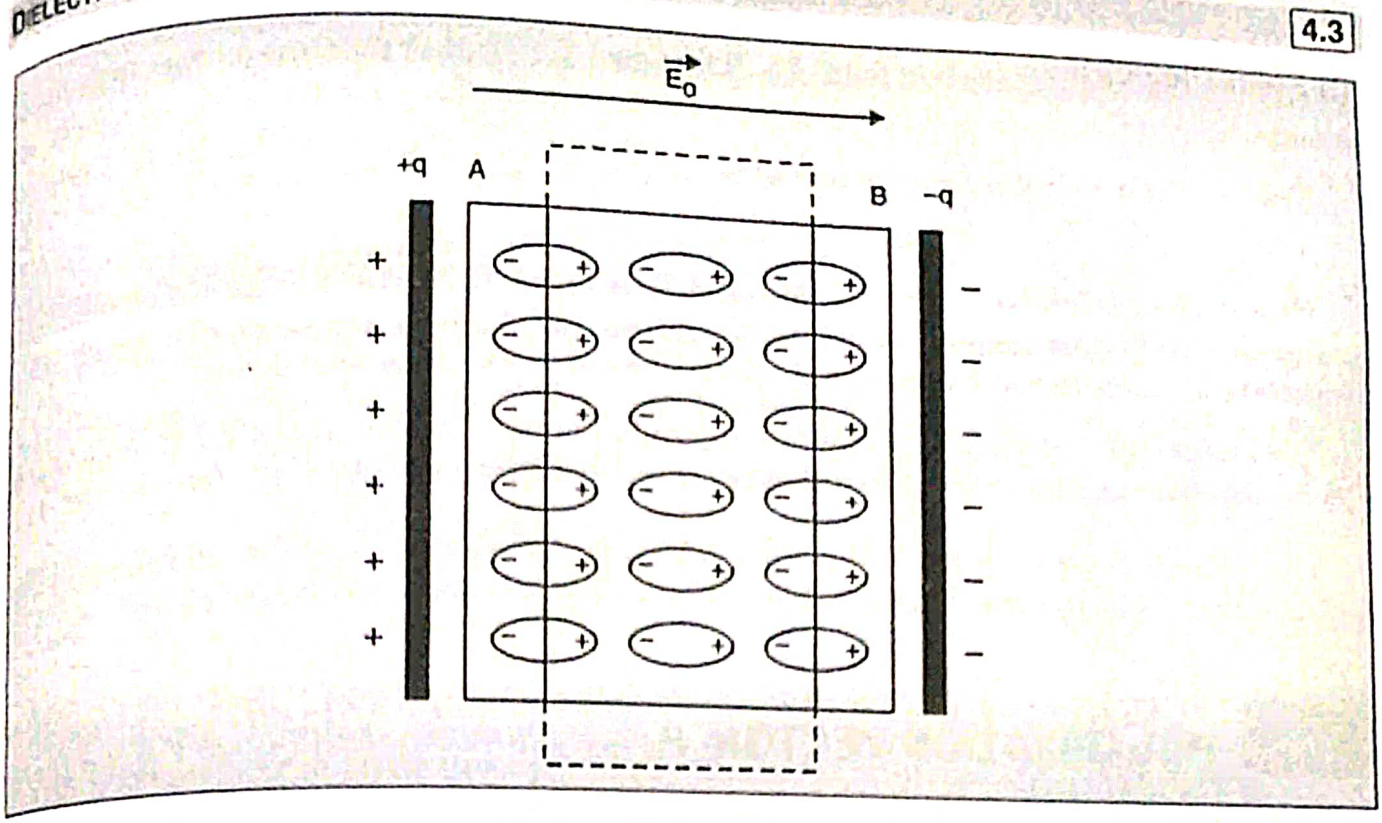


Fig. 4.4

Consider a dielectric slab placed in an external electric field between the plates of a charged parallel plate capacitor. Let strength of electric field between the plates is $\vec{E_0}$. The presence of external electric field will shift the centers of gravity of positive and negative charges of the molecules (in opposite directions) in case of non polar dielectric thus converting non-polar molecules is to polar molecules. If the dielectric consists of polar molecules, then in addition of shifting the centres of gravity of positive and negative charges (in opposite direction), it will also break the close chains of electric dipoles. The centres of gravity of negative charges will shift towards positive plate and centres of gravity of positive charges towards negative plate of the capacitor. This will result in alignment of electric dipoles along the direction of electric field. The positive charge of the molecule inside the dielectric is followed by the negative charge of next molecule and so on as shown in Fig. (4.4). Since the molecules are very close, hence positive charge on molecule is cancelled by the negative charge of next adjacent molecule and so on. Hence the net charge within the dielectric is zero except near the surfaces of the dielectric.

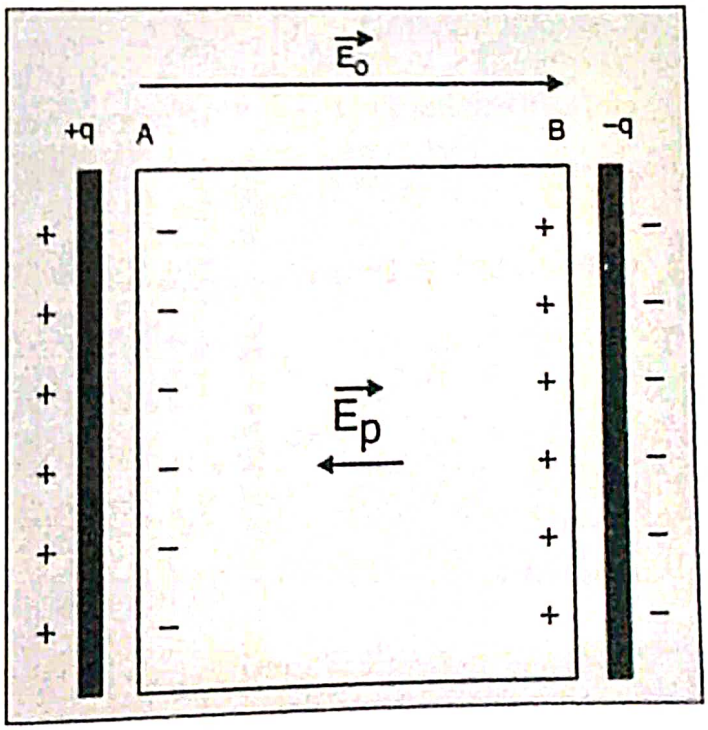


Fig. 4.5

Net negative charge will appear on surface A and net positive charge on surface B of the dielectric as shown in Fig. (4.5). The appearance of the net negative and positive charges on the opposite faces of dielectric produces an electric field $\vec{E_p}$, within dielectric. Thus field acts in the direction

opposite to the applied electric field $\vec{E_0}$. Therefore net electric field inside the dielectric is reduced.

The net electric field inside the dielectric will be

$$E = E_0 - E_p \qquad \ldots(4.2)$$

Hence when a dielectric slab is placed in an electric field, the strength of electric field gets reduced. **The phenomena of appearance of charges on opposite faces of a dielectric slab, induced by external electric field is called polarization.**

The charges on the surface of plates of a parallel plate capacitor are called **free charges.** The surface density due to these free charges is called surface density of the free charges σ_f.

The induced charges on the surface of a polarized dielectric are called bound charges. The surface density due to these bound charges is called surface density of bound charges σ_p.

4.4 POLARIZATION VECTOR $\vec{P}$

The induced dipole moment per unit volume of a dielectric is called polarization vector $\vec{P}$.

Let induced dipole moment of the dielectric = $\vec{p_i}$.

Volume of dielectric = V

Then polarization vector

$$\vec{P} = \frac{\vec{p_i}}{V}$$

$$\therefore \quad \vec{P} = \frac{q_i \vec{d}}{V} \qquad \text{where } \vec{p_i} = q_i \vec{d}$$

and d = thickness of slab

The direction of $\vec{P}$ is form $-q_i$ to q_i

Magnitude of polarization vector

$$P = \frac{q_i d}{V}$$

Or $$P = \frac{q_i d}{Ad} \qquad (\because V = Ad)$$

Where A is area of surface of dielectric

$$\therefore \quad P = \frac{q_i}{A} = \sigma_p \qquad \ldots(4.3)$$

Hence polarization of a dielectric is numerically equal to the surface density of bound charge

The *SI* units of P are $\frac{C}{m^2}$.

4.5 SUSCEPTIBILITY

The polarization of a dielectric is caused by the electric field. So polarization density is directly proportional to the product of net electric field $\vec{E}$ inside the dielectric and electric permittivity of free space

$$\vec{P} \propto \epsilon_0 \vec{E}$$

or

$$\vec{P} = \epsilon_0 \chi_e \vec{E} \qquad \ldots(4.4)$$

where χ_e is called electric susceptibility of the dielectric (and $\vec{E} = \vec{E}_0 - \vec{E}_p$).

ϵ_0 is permittivity of air or vacuum.

or

$$P = \epsilon_0 \chi_e E$$

$$\therefore \quad \chi_e = \frac{P}{\epsilon_0 E} \qquad \ldots(4.5)$$

From eq. (4.5), the susceptibility χ_e has no units and it is dimensionless.

4.6 DIELECTRIC CONSTNANT

Consider a parallel plate capacitor with air (or vacuum) as medium between two plates. Let charges on two plates are $+q$ and $-q$.

Let uniform electric field between the plates of the capacitor is $\vec{E}_0$ as shown in Fig. (4.6).

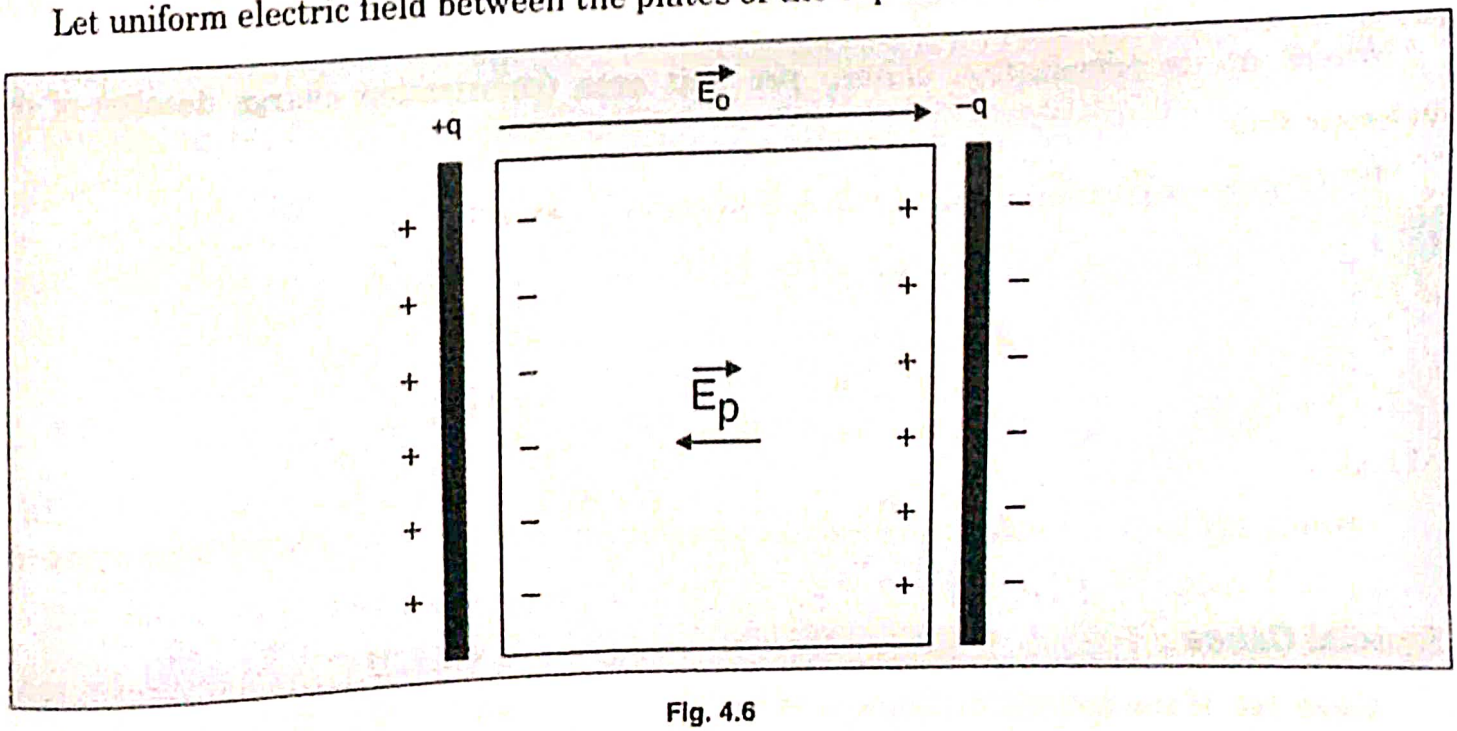


Fig. 4.6

Now introduce a dielectric slab between the plates of the capacitor. The dielectric gets polarized and net electric field inside the dielectric is given by

$$E = E_0 - Ep \qquad \ldots(4.6)$$

Where E_p is the electric field produced inside the dielectric due to induced charges as shown in Fig. (4.6).

The ratio of the electric field inside the capacitor without dielectric to the electric field inside the capacitor with dielectric is called dielectric constant. It is denoted by K.

Thus dielectric constant

$$K = \frac{E_0}{E}$$

or $$K = \frac{E_0}{E_0 - E_p} \qquad \text{using eq. (4.6)} \ldots(4.7)$$

As $$E_0 > E_p$$

$\therefore$ $$K > 1$$

Since electric field between the plates of capacitor with air (or vacuum) as medium is given by

$$E_0 = \frac{\sigma_f}{\epsilon_0} \qquad \ldots(4.8)$$

Where σ_f is surface density due to free charges on plates of the capacitor.

Also electric field due to induced (bound) charges inside the dielectric.

$$E_p = \frac{\sigma_p}{\epsilon_0} \qquad \ldots(4.9)$$

Where σ_p is polarization charge per unit area (polarization charge density) of the dielectric slab.

Putting the values from eqs. (4.8 & 4.9) in eq. (4.7), we get

$$K = \frac{\frac{\sigma_f}{\epsilon_0}}{\frac{\sigma_f}{\epsilon_0} - \frac{\sigma_p}{\epsilon_0}}$$

or $$K = \frac{\sigma_f}{\sigma_f - \sigma_p} \qquad \ldots(4.10)$$

Special Cases

Case Ist. If the dielectric sample is of metal

$$\sigma_p = \sigma_f$$

i.e.

$$K = \infty$$

Then

It means metal has infinite dielectric constant

Case IInd. If the dielectric is vacuum

$$\sigma_p = 0$$

i.e.

$$K = 1$$

Then

Thus dielectric constant of vacuum is one.

Let capacity of the capacitor with vacuum or air (without dielectric) = C_0

Potential difference between the plates of the capacitor with air as medium.

$$V_0 = E_0 d \qquad \ldots(4.11)$$

Where d is distance between the plates of the capacitor

$$C_0 = \frac{q}{V_0} \qquad \ldots(4.12)$$

or

$$C_0 = \frac{q}{E_0 d} \qquad \ldots(4.13) \text{ [using eq. (4.11)]}$$

Let the capacity of the capacitor with dielectric slab between the plates = C.

Potential difference between the plates of the capacitor (with dielectric) = V

Then

$$V = Ed \qquad \ldots(4.14)$$

and

$$C = \frac{q}{V}$$

or

$$C = \frac{q}{Ed} \qquad \ldots(4.15) \text{ [using eq. (4.14)]}$$

Dividing eq. (4.15) by eq. (4.13), we get

$$\frac{C}{C_0} = \frac{\frac{q}{Ed}}{\left(\frac{q}{E_0 d}\right)} = \frac{E_0}{E} \qquad \ldots(4.16)$$

Since

$$E_0 > E \qquad \ldots(4.17)$$

$$\therefore \quad C > C_0$$

Hence capacity of a capacitor increases on introducing a dielectric between the plates.

Dividing eq. (4.11) by eq. (4.14), we get

$$\frac{V_0}{V} = \frac{E_0 d}{Ed}$$

$$\frac{V_0}{V} = \frac{E_0}{E} \quad \text{...(4.18)}$$

or

Since $E_0 > E$

$\therefore$ $V_0 > V$ ...(4.19)

Hence potential of a capacitor decreases on introducing a dielectric slab.

4.7 RELATION BETWEEN DIELECTRIC CONSTANT AND SUSCEPTIBILITY

Consider a charged parallel plate capacitor with vacuum (or air) as medium between the plates of the capacitor.

Let charge on the capacitor = q

Surface charge density of the plates of capacitor = σ_f.

The uniform electric field between the plates of capacitor is given by

$$E_0 = \frac{\sigma_f}{\epsilon_0}$$

Now introduce a dielectric slab between the plates of the capacitor. The dielectric slab gets polarized and the net electric field inside the dielectric is given by

$$E = E_0 - E_p \quad \text{...(4.20)}$$

Where E_p is the electric field produced inside the dielectric slab due to induced charges (or bound charges) as shown in Fig. (4.6).

Then $$E_p = \frac{\sigma_p}{\epsilon_0}$$

Where σ_p is surface density due to induced (or bound) charges.

Putting this value in eq. (4.20), we get

$$E = E_0 - \frac{\sigma_p}{\epsilon_0} \quad \text{...(4.21)}$$

We know that polarization of dielectric

$$P = \sigma_p \quad \text{using eq. (4.3)}$$

Putting this value in Eq. (4.21), we get

$$E = E_0 - \frac{P}{\epsilon_0} \quad \text{...(4.22)}$$

Dividing both sides by E

$$\frac{E}{E} = \frac{E_0}{E} - \frac{P}{\epsilon_0 E}$$

$$1 = \frac{E_0}{E} - \frac{P}{\epsilon_0 E}$$

or ...(4.23)

Since dielectric constant

$$K = \frac{E_0}{E}$$

and electric susceptibility of dielectric

$$\chi_e = \frac{P}{\epsilon_0 E}$$ using eq. (4.5)

Putting these values in eq. (4.23), we get

$$1 = K - \chi_e$$

$$K = 1 + \chi_e$$

or ...(4.24)

This is the relation between dielectric constant K and electric susceptibility of a dielectric.

4.8 RELATION BETWEEN $\vec{E}$, $\vec{P}$ AND $\vec{D}$

Consider the polarization of a dielectric slab between the plates of a charged parallel plate capacitor.

Let σ_f is the surface charge density of free charges on the plates of the capacitor.

σ_p is surface density of bound (or polarization) charges. Then magnitude of electric field between the plates of charged capacitor (with air as medium).

$$E_0 = \frac{\sigma_f}{\epsilon_0}$$ ...(4.25)

Magnitude of electric field inside the dielectric due to induced charges.

$$E_p = \frac{\sigma_p}{\epsilon_0}$$ ..(4.26)

Net electric field inside the dielectric is

$$E = E_0 - E_p$$

or $$E_0 = E + E_p$$ ...(4.27)

or $$E_0 = E + \frac{\sigma_p}{\epsilon_0}$$ using eq. (4.26)

or $$\epsilon_0 E_0 = \epsilon_0 E + \sigma_p$$

or $$\epsilon_0 E_0 = \epsilon_0 E + P$$ ($\because P = \sigma_p$)

or $$\epsilon_0 \frac{\sigma_f}{\epsilon_0} = \epsilon_0 E + P$$ using eq. (4.25)

or $$\sigma_f = \epsilon_0 E + P \quad \ldots(4.28)$$

Let $$\sigma_f = D$$

where $\vec{D}$ is electric displacement vector.

Then eq. (4.28) becomes

$$D = \epsilon_0 E + P \quad \ldots(4.29)$$

In vector form

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P} \quad \ldots(4.30)$$

Relation between $\vec{D}$ and $\vec{E}$

Since $$D = \sigma_f = \frac{q}{A} \quad \ldots(4.31)$$

where A = Area of each plate of capacitor

Electric field between plates of capacitor with dielectric in between the plates

$$E = \frac{q}{\epsilon_0 KA}$$ where K is dielectric constant

or $$q = \epsilon_0 EKA$$

Putting this value in eq. (4.31)

$\therefore$ $$D = \frac{\epsilon_0 KAE}{A}$$

or $$D = (\epsilon_0 K)E$$

or $$D = \epsilon E \quad (\because \epsilon = \epsilon_0 k)$$

where ϵ is permittivity of dielectric

or $$\vec{D} = \epsilon \vec{E} \quad \ldots(4.32)$$

The units of $\vec{D}$ is Cm^{-2}

Units of $\vec{P}$ is also Cm^{-2}

Relation between $\vec{P}$ and $\vec{E}$

From eq. (4.21)

$$E_0 = E + \frac{P}{\epsilon_0}$$

$$\epsilon_0 E_0 = \epsilon_0 E + P$$

or

$$K = \frac{E_0}{E} \qquad \text{...(4.33)}$$

Since

$$E_0 = KE$$

or

Putting this value in eq. (4.33), we get

$$\epsilon_0 KE = \epsilon_0 E + P$$

$$P = \epsilon_0 KE - \epsilon_0 E$$

or

$$P = \epsilon_0 (K-1) E$$

or ...(4.34)

If no dielectric is present i.e. $K = 1$

Then

$$P = 0$$

Which is correct because in the absence of dielectric, there is no polarization.

Since $K - 1 = \chi_e$ using e.g. (4.24)

$\therefore$ Eq. (4.34), becomes

$$P = \epsilon_0 \chi_e E \qquad \text{...(4.35)}$$

Where χ_e is electric susceptibility of dielectric.

4.9 ATOMIC POLARIZABILITY

When a non-polar atom is placed in an electric field, it becomes induced electric dipole and has induced dipole moment. The process of producing induced dipole is called polarization of atom. It has been found that dipole moment induced is directly proportional to strength of applied electric field.

i.e. $p \propto E_0$

or $p = \propto E_0$

where $\propto$ is a constant of proportionality called **polarizability of atom.**

$$\propto = \frac{p}{E_0} \qquad \text{...(4.36)}$$

Consider an atom of atomic number Z having spherically symmetric charge distribution of radius r. In the absence of electric field atom is non-polar we assume that in the absence of electric field, whole of the positive charge is concentrated at the centre of the atom (i.e. at the nucleus) and negative charge is spread around in the form of spherical cloud as shown in Fig. (4.7).

Let this atom is now placed in an electric field E_0 (i.e. polarizing field). The positive and negative charges will experience force, due to this electric field, in opposite directions. Since the positive charge is concentrated in the nucleus and due to its large mass its position remains fixed, but negative charge cloud is displaced towards the positive plate of the charged capacitor as shown in Fig. 4.8. Let distance between the centres of positive and negative charges = x. The force acting on the positive charge due to applied electric field (i.e. towards negative plate of the capacitor), is

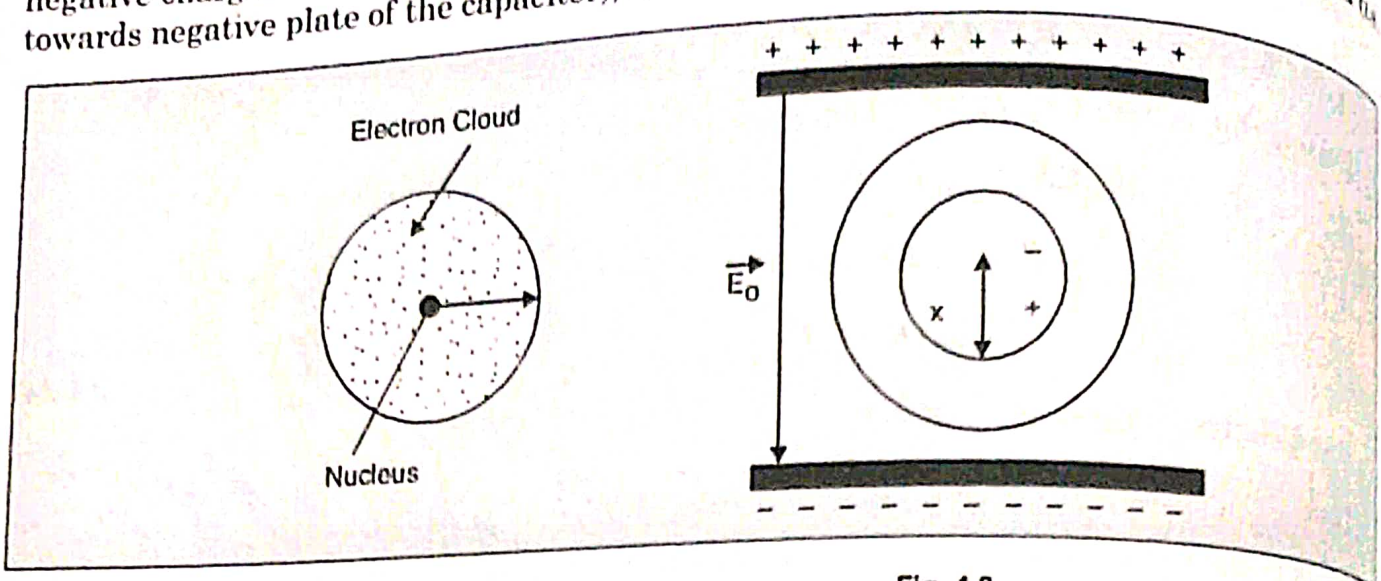


Fig. 4.7 Fig. 4.8

$$F = qE_0 = ZeE_0 \quad \ldots(4.37)$$

Where charge on the nucleus is Ze.

The force on positive charge (i.e. towards negative plate) is balanced by the force due to negative charge ($-Ze$) cloud contained in a sphere of radius x.

Let volume charge density of atom = ρ

The electronic charge in volume $\frac{4}{3}\pi r^3 = Ze$

$\therefore$ Electronic charge per unit volume = $\dfrac{Ze}{\frac{4}{3}\pi r^3}$

The electronic charge in a sphere of volume $\frac{4}{3}\pi x^3$ is

$$q = \frac{Ze}{\frac{4}{3}\pi r^3} \times \frac{4}{3}\pi x^3$$

$$\therefore \quad q = \frac{Zex^3}{r^3} \quad \ldots(4.38)$$

From Coomb's law the electrostatic force of attraction between the nucleus and electron cloud is

$$F' = \frac{1}{4\pi\epsilon_0}\frac{(Ze)q}{x^2}$$

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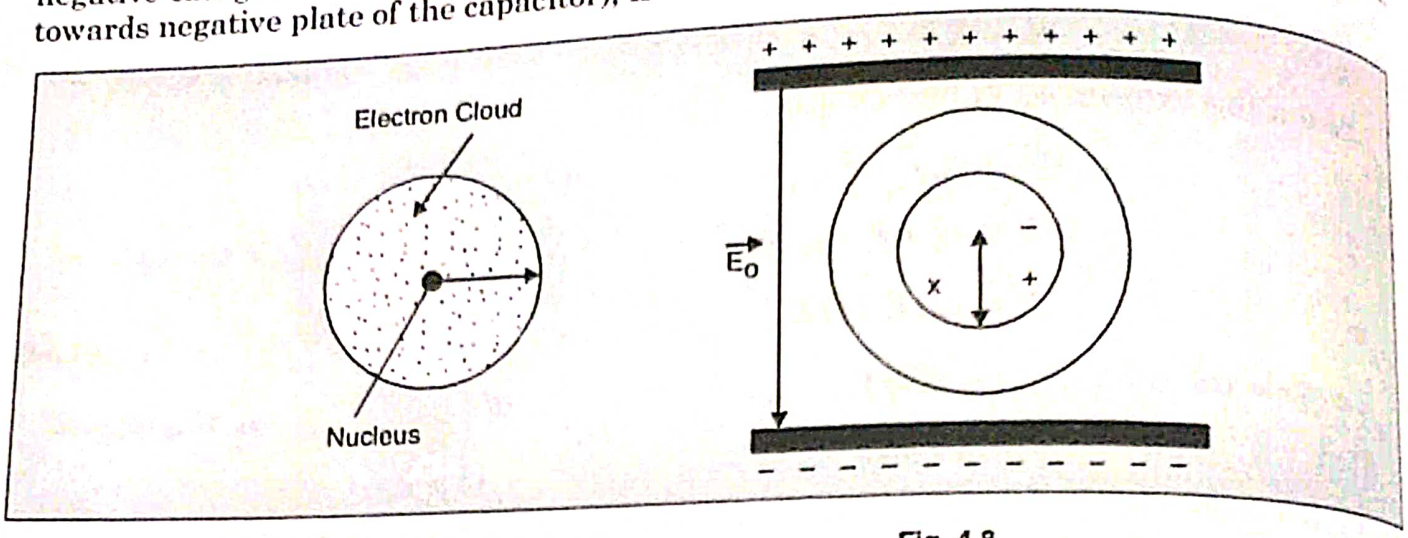

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From Coomb's law the electrostatic force of attraction between the nucleus and electron cloud is

$$F' = \frac{1}{4\pi\epsilon_0}\frac{(Ze)q}{x^2}$$

or $$F' = \frac{1}{4\pi \epsilon_0} \frac{(Ze)}{x^2} \left(\frac{Ze\, x^3}{r^3} \right)$$ using eq. (4.38)

or $$F' = \frac{1}{4\pi \epsilon_0} \frac{(Ze)^2 x}{r^3} \quad \ldots(4.39)$$

In equilibrium

$$F = F'$$

$\therefore$ $$(Ze)\, E_0 = \frac{1}{4\pi \epsilon_0} \frac{(Ze)^2 x}{r^3}$$

or $$E_0 = \frac{(Ze)x}{4\pi \epsilon_0 r^3}$$

or $$E_0 = \frac{p}{4\pi \epsilon_0 r^3} \quad \ldots(4.40)\ [\because (Ze)x = p]$$

or $$\frac{p}{E_0} = 4\pi \epsilon_0 r^3$$

So polarizability $\alpha = 4\pi \epsilon_0 r^3$ [using eq. (4.36)]

$\therefore$ Eq. (4.40) can be written as

$$p = \alpha E_0$$

In vector form

$$\vec{p} = \alpha \vec{E}_0 \quad \ldots(4.41)$$

If there are n atoms per unit volume, then

Polarization density $\vec{P} = n \vec{p} = n \alpha \lambda . \vec{E}_0$

The units of atomic polarizability

$$\alpha = \frac{\text{Dipole moment}}{\text{Electric field}} = \frac{Cm}{Vm^{-1}} = \frac{Cm^2}{V} = \text{Farad metre}^2$$

$$= Fm^2$$

4.10 NON-UNIFORM POLARIZATION OF DIELECTRIC

Consider a non isotropic and inhomogeneous dielectric. In such dielectric the dielectric constant k and polarization vector $\vec{P}$ are not constant. Place this dielectric in a non-uniform electric field. Then different parts of the dielectric would be polarized differently or it would have non-uniform polarization. Let this dielectric is of area vector $\vec{S}$ and volume V. In such

dielectric the charges move in certain direction will be more than charges moving away from this region.

Let ρ_p and σ_p be respectively, the volume charge density and surface charge density of the induced charge. Although such movement of charges due to polarization may not affect σ_p but it will certainly affect ρ_p.

Consider a small volume element dV of area dS of the dielectric.

Then net charge due to polarization (induced charge) is given as

$$q_p = -\iint_S \sigma_p \, dS \qquad \ldots(4.42)$$

The negative sign shows that polarization charge q_p is in opposite direction to that of surface charge density σ_p.

Since $\sigma_p = \vec{P}.\vec{n}$

Putting this value in eq. (4.42), we get

$$q_p = -\iint_S \vec{P}.\hat{n}\, dS$$

where $\hat{n}$ is unit vector along area vector

or $$q_p = -\iint_S \vec{P}.d\vec{S} \qquad \ldots(4.43)\ (\because \hat{n}\, dS = d\vec{S})$$

Also q_p in terms of volume charge density is given as

$$q_p = \iiint_V \rho_p dV \qquad \ldots(4.44)$$

From eqs. (4.43 & 4.44)

$$\iint \vec{P}.d\vec{S} = -\iiint_V \rho_p dV \qquad \ldots(4.45)$$

Using Gauss Divergence theorem

$$\iint \vec{P}.d\vec{S} = \iiint_V \vec{\nabla}.\vec{P}\, dV \qquad \ldots(4.46)$$

From eqs. (4.45 & 4.46), we get

$$\iiint_V \vec{\nabla}.\vec{P}\, dV = -\iiint_V \rho_p \, dV$$

or $$\vec{\nabla}.\vec{P} = -\rho_p \qquad \ldots(4.47)$$

Since in non-uniform polarization $\vec{P}$ is not constant, hence $\vec{\nabla}.\vec{P} \neq 0$.

In case of uniform polarization $\vec{P}$ is constant. Hence $\vec{\nabla}.\vec{P} = 0$.

4.11 LOCAL FIELD AT AN ATOM

In dielectrics, an atom or molecule when placed in an external electric field, experiences not only the external field but also the fields produced by dipoles. As a result of long range coulomb forces, the contribution of latter cannot be neglected. The **resultant field responsible for polarizing individual molecules or atoms of solids (dielectrics) is called the local field.**

Let us calculate the local field by method suggested by Lorentz. Consider a dielectric slab is placed between the plates of a charged parallel plate capacitor. Now consider a spherical cavity with dimensions greater than molecular dimensions within the dielectric. As the polarization takes place, let the surface charge density (charge per unit area) of capacitor plates = σ_f.

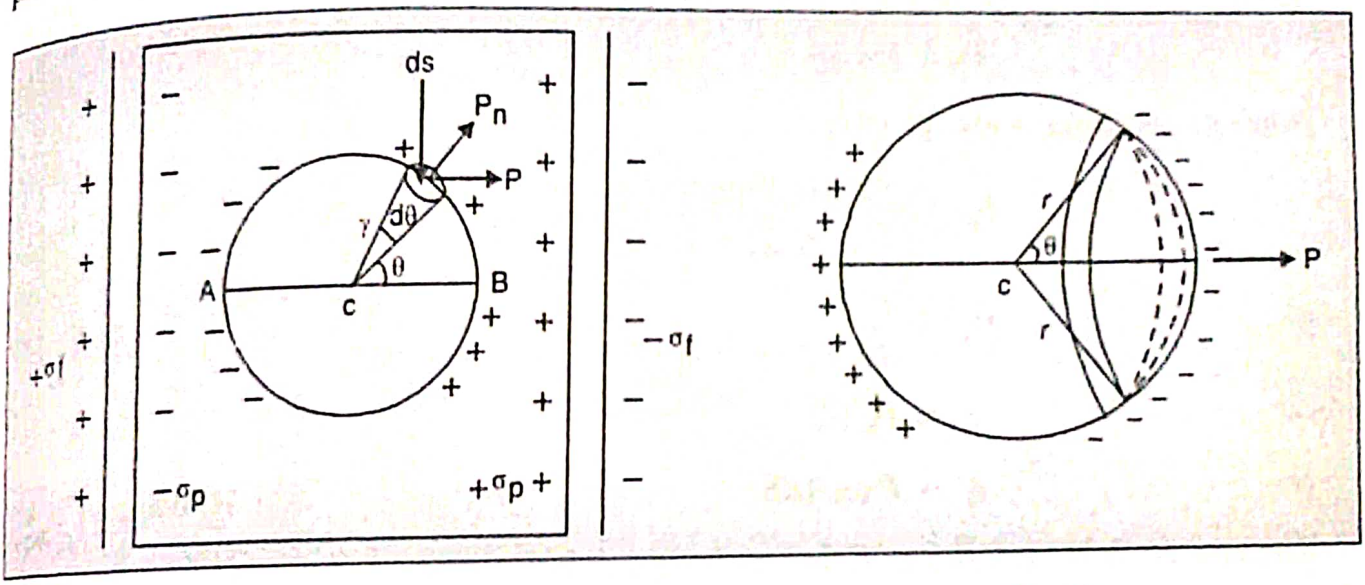


Fig. 4.9

Fig. 4.10

The surface charge density of cavity due to polarized charges = σ_p.

Consider the molecle at centre C of the cavity as shown in Fig. (4.9). Then net field (local field) experienced by it is given as

$$E_{loc} = E_0 + E_p + E_s + E_m \qquad \ldots(4.48)$$

where E_0 is the field between two plates of capacitor without dielectric. So

$$E_0 = \frac{\sigma_f}{\epsilon_0}$$

E_p is field at C due to polarized charges on plane surfaces of dielectric. So

$$E_p = \frac{\sigma_p}{\epsilon_0}$$

E_s is the field at C due to polarized charges on the surface of cavity to be calculated.

E_m is the field at C due to all the dipoles of the atoms inside the spherical cavity. In case of non-polar isotropic dielectric, it is zero

i.e. $$E_m = 0$$

Putting these values in eq. (4.48), we get

$$E_{loc} = \frac{\sigma_f}{\epsilon_0} + \frac{\sigma_p}{\epsilon_0} + E_s$$

$$E_{loc} = E + E_s \qquad \ldots(4.49)\ (\because E = E_0 + E_p)$$

where E is resultant electric field between the plates.

Let us calculate E_s. Consider a small area element dS on the surface of cavity (making a solid angle $d\theta$ at C) at an angle θ with the direction of electric field E. The direction of polarization P will be parallel to E.

The component of P perpendicular to dS is given as

$$P_N = P\cos\theta \qquad \ldots(4.50)$$

Since polarization is also given as

$$P_N = \frac{\text{Surface Charge}}{\text{Area}}$$

or $$P_N = \frac{q'}{dS}$$

or $$q' = P_N\, dS$$

or $$q' = P\cos\theta\, dS \qquad \ldots(4.51) \text{ using eq. (4.50)}$$

The electric field intensity at C due to charge q' is given as

$$dE_s = \frac{1}{4\pi\epsilon_0}\frac{q'}{r^2} \qquad \text{(where } r \text{ is radius of cavity)}$$

or $$dE_s = \frac{1}{4\pi\epsilon_0}\frac{P\cos\theta\, dS}{r^2} \qquad \ldots(4.52) \text{ using eq. (4.51)}$$

This field intensity is along r.

Now resolving dE_s into components parallel and perpendicular to P.

The component of dE_s parallel to P

$$= \frac{1}{4\pi\epsilon_0}\frac{P\cos\theta\, dS}{r^2}\cos\theta$$

$$= \frac{1}{4\pi\epsilon_0}\frac{P\cos^2\theta\, dS}{r^2} \qquad \ldots(4.53)$$

The component of dE_s perpendicular to P

$$= \frac{1}{4\pi \epsilon_0} \frac{P \cos\theta dS}{r^2} \sin\theta$$

$$= \frac{1}{4\pi \epsilon_0} \frac{P \sin\theta \cos\theta}{r^2} dS$$

We see that the perpendicular components will be cancelled due to an equal contribution from another symmetrically situated surface elements. The only components along the direction of P will contribute to the integral of eq. (4.53) over the entire surface

$$\therefore \quad E_s = \iint_S \frac{1}{4\pi \epsilon_0} \frac{P \cos^2\theta dS}{r^2} \qquad \ldots(4.54)$$

Now the appropriate surface element dS in this case is a ring. So that

$$dS = 2\pi r \sin\theta r d\theta = 2\pi r^2 \sin\theta d\theta$$

and the limits of integration with respect to θ are from 0 to π as shown in Fig. (4.10)

Thus eq. (4.54) becomes

$$E_s = \int_0^{\pi} \frac{1}{4\pi \epsilon_0} \frac{P \cos^2\theta}{r^2} 2\pi r^2 \sin\theta d\theta$$

or

$$E_s = \frac{1}{2 \epsilon_0} \int_0^{\pi} P \sin\cos^2\theta d\theta \qquad \ldots(4.55)$$

Put $x = \cos\theta$

Then $dx = -\sin\theta \, d\theta$

Putting these values in eq. (4.55), we get

$$E_s = -\frac{1}{2 \epsilon_0} \int_1^{-1} P x^2 dx$$

$$= -\frac{1}{2 \epsilon_0} P \int_1^{-1} x^2 dx = \frac{-P}{2 \epsilon_0} \left[\frac{x^3}{3}\right]_1^{-1} = -\frac{P}{6 \epsilon_0} \left[x^3\right]_1^{-1}$$

$$= -\frac{P}{6 \epsilon_0} \left[(-1)^3 - (1)^3\right] = -\frac{P}{6 \epsilon_0} [-1 - 1]$$

$$E_s = -\frac{P}{6 \epsilon_0} (-2) = \frac{P}{3 \epsilon_0} \qquad \ldots(4.56)$$

Putting this value in eq. (4.49), we get

$$E_{loc} = E + \frac{P}{3\epsilon_0} \quad \ldots(4.57)$$

This eq. (4.57) shows that E_{loc} is different from E. The former field is larger than the latter, so the molecules are more effectively polarized than our earlier study. This eq. (4.57) is known as Lorentz relation.

4.12 CLAUSIUS MOSOTTI EQUATION

In order to correlate the macroscopic properties of dielectric and microscopic properties of atoms Clausius and Mosotti derived a relation between dielectric constant (i.e. macroscopic parameter) and atomic polarizability (i.e. microscopic parameter) called Clausius Mosotti equation.

When an isotropic non-polar dielectric is placed in an external electric field, it experiences not only the external field but also the fields produced by dipoles. As a result of long range coloumb forces, the contribution of latter cannot be neglected. The resultant field responsible for polarizing individual molecules or atoms of dielectric is called the local field. Local field at an atom is given as

$$\vec{E}_{loc} = \vec{E} + \frac{\vec{P}}{3\epsilon_0} \quad \ldots(4.58) \text{ using eq. (4.57)}$$

where P is polarization and $E = E_0 + E_p$

Let $\vec{p}$ be the electric dipole moment of each atom, then

$$\vec{p} \propto \vec{E}_{loc}$$

or $$\vec{p} = \propto \vec{E}_{loc}$$

where α is atomic polarizability

Let number of atoms per unit volume of dielectric = n

$\therefore$ Polarization per unit volume is

$$\vec{P} = n\vec{p}$$

or $$\vec{P} = n\alpha E_{loc} \quad \ldots(4.59)$$

or $$\vec{P} = n\alpha\left[\vec{E} + \frac{\vec{P}}{3\epsilon_0}\right] \quad \text{using eq. (4.58)}$$

$$\frac{\vec{P}}{n\alpha} = \vec{E} + \frac{\vec{P}}{3\epsilon_0}$$

or ...(4.60)

The displacement vector is given as

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P}$$

...(4.61) using eq. (4.30)

Also displacement vector is given as

$$\vec{D} = \epsilon_0 K \vec{E}$$

using eq. (4.32)

where K is dielectric constant

Putting this value in eq. (4.61)

$$\epsilon_0 K \vec{E} = \epsilon_0 \vec{E} + \vec{P}$$

or $$\epsilon_0 K \vec{E} - \epsilon_0 \vec{E} = \vec{P}$$

or $$\epsilon_0 (K-1) \vec{E} = \vec{P}$$

or $$\vec{E} = \frac{\vec{P}}{\epsilon_0 (K-1)}$$ ...(4.62)

Putting the is value in eq. (4.60), we get

$$\frac{\vec{P}}{n\alpha} = \frac{\vec{P}}{\epsilon_0 (K-1)} + \frac{\vec{P}}{3\epsilon_0}$$

$$= \frac{\vec{P}}{\epsilon_0}\left[\frac{1}{K-1} + \frac{1}{3}\right]$$

$$= \frac{\vec{P}}{\epsilon_0}\left[\frac{3+K-1}{3(K-1)}\right]$$

$$= \frac{\vec{P}}{\epsilon_0}\left[\frac{K+2}{3(K-1)}\right]$$

$\therefore$ $$\frac{\vec{P}}{n\alpha} = \frac{\vec{P}}{3\epsilon_0}\left[\frac{K+2}{K-1}\right]$$

or $$\frac{1}{n\alpha} = \frac{1}{3\epsilon_0}\left(\frac{K+2}{K-1}\right)$$

or $$\boxed{\alpha = \frac{3\epsilon_0}{n}\left(\frac{K-1}{K+2}\right)}$$ ...(4.63)

This equation is called Clausius-Mosotti Equation. If we use symbol ϵ_r for k, then eq (4.63) can be written as

$$\alpha = \frac{3\epsilon_0}{n}\left(\frac{\epsilon_r - 1}{\epsilon_r + 2}\right) \quad \ldots(4.64)$$

4.13 CLASSICAL THEORY OF ELECTRONIC POLARIZABILITY

Electronic probability arises due to relative displacement of nucleus and electrons within the atom.

When an electric field is applied to a molecule, the individual atoms in the molecule get polarized. The electrons in the various shells are displaced relative to the nucleus produce an electric dipole moment as shown in Fig. 4.11.

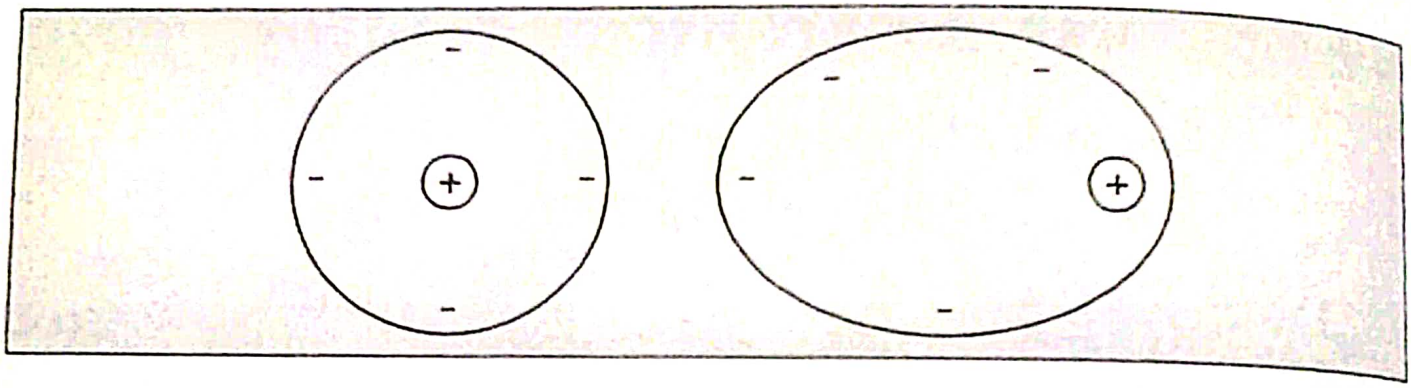


Fig. 4.11

Thus every atom in a crystal has electronic polarizability.

In order to find the expression for electronic polarizability, we can predict that the restoring force on the electron cloud, when displaced from normal configuration about the nucleus is proportional to displacement. Thus the system can be approximated with a harmonic oscillator. As a result, equation of motion of an electron bound harmonically to an atom in an oscillating field $E_e e^{i\omega t}$ can be written as

$$\frac{md^2x}{dt^2} + m\gamma\frac{dx}{dt} + m\omega_0^2 x = e E_0 e^{i\omega t} \quad \ldots(4.65)$$

where m is mass of electron, ω_0 natural frequency of oscillation of electron, w the frequency of applied field, e is charge on electron and γ includes damping effects. It is related to natural frequency as

$$\gamma = \frac{\mu_0 e^2 \omega_0^2}{6\pi mc}$$

where $c = 3\times10^8$ m/s and $\mu_0 = 1.257\times10^{-6}$ h/m.

If the solution of equation (4.65) is

$$x = x_0 e^{i\omega t}$$

Then $$\frac{dx}{dt} = i\omega x_0 e^{i\omega t} = i\omega x$$

and $$\frac{d^2x}{dt^2} = -\omega^2 x_0 e^{i\omega t} = -\omega^2 x$$

Putting these values in eq. (4.65), we get

$$-m\omega^2 x + im\gamma\omega x + m\omega_0^2 x = e E_0 e^{i\omega t}$$

or $$mx(-\omega^2 + i\omega\gamma + \omega_0^2) = e E_0 e^{i\omega t}$$

or $$x = \frac{e}{m} \frac{E_0 e^{i\omega t}}{(\omega_0^2 - \omega^2 + i\omega\gamma)} \quad \ldots(4.66)$$

The electronic polarizability is given as

$$\alpha_e = \frac{ex}{E_0 e^{i\omega t}}$$

or $$\alpha_e = \frac{e^2}{m(\omega_0^2 - \omega^2 + i\omega\gamma)} \quad \ldots(4.67) \text{ using eq. (4.66)}$$

This is the required expression of electric polarizability. The complex dielectric constant is given as

$$\epsilon_r(\omega) = 1 + \chi_e \quad \ldots(4.68)$$

Since χ_e is proportional to α_e

$\therefore$ χ_e can be written as

$$\chi_e = N\alpha_e$$

where N is constant of proportionality and equal to number of electrons per unit volume

$\therefore$ $$\chi_e = \frac{Ne^2}{m(\omega_0^2 - \omega^2 + i\omega\gamma)} \quad \text{using eq. (4.67)}$$

Putting this value in eq. (4.68), we get

$$\epsilon_r(\omega) = 1 + \frac{Ne^2}{m(\omega_0^2 - \omega^2 + i\omega\gamma)}$$

$$= 1 + \frac{Ne^2}{m[(\omega_0^2 - \omega^2) + i\omega\gamma)]} \times \frac{(\omega_0^2 - \omega^2) - i\omega\gamma}{(\omega_0^2 - \omega^2) - i\omega\gamma}$$

$$= 1 + \frac{Ne^2}{m} \frac{(\omega_0^2 - \omega^2)}{[(\omega_0^2 - \omega^2)^2 + \omega^2\gamma^2]} - \frac{iNe^2}{m} \frac{\omega\gamma}{[(\omega_0^2 - \omega^2)^2 + \omega^2\gamma^2]}$$

$$\epsilon_r(\omega) = 1 + \epsilon_r'(\omega) - i\epsilon_r''(\omega) \quad \ldots(4.69)$$

where $$\epsilon_r'(\omega) = \frac{Ne^2}{m} \frac{(\omega_0^2 - \omega^2)}{[(\omega_0^2 - \omega^2)^2 + \omega^2\gamma^2]} \quad \ldots(4.70)$$

and $$\epsilon_r''(\omega) = \frac{Ne^2}{m} \frac{\gamma\omega}{[(\omega_0^2 - \omega^2)^2 + \omega^2\gamma^2]} \quad \ldots(4.71)$$

Here $\epsilon_r'(\omega)$ gives the value of dielectric constant and $\epsilon_{r(\omega)}''$ gives information about damping losses.

The variation of ϵ_r' with frequency and ϵ_r'' with frequency are shown in Figs. (4.12 & 4.13).

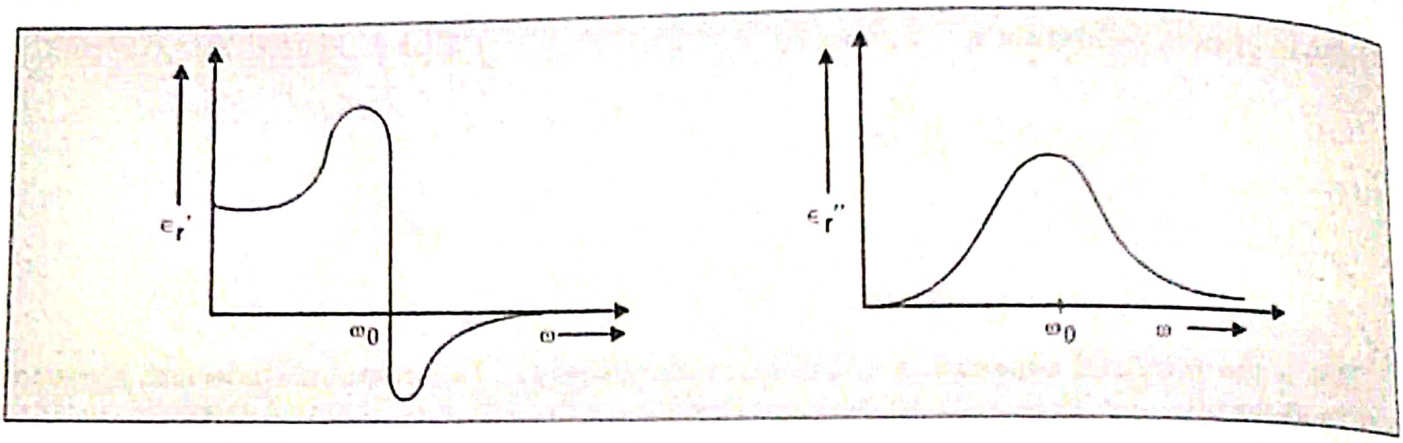


Fig. 4.12 Fig. 4.13

As shown in Fig. (4.13) ϵ_r'' has maximum value at $\omega = \omega_0$. The meaning of this maximum is that material absorbs energy at natural frequency. This phenomenon is called "resonance absorption". ϵ_r' is strongly frequency dependent and the susceptibility undergoes a change in sign in this region. This phenomenon is called "anomalous dispersion."

4.14 TYPES OF POLARIZATION

There are four different atomic mechanism by which electrical polarization can occur in dielectric materials when they are subjected to an external electric field. Polarization are mainly of following types.

(i) Electronic polarization.

(ii) Ionic polarization.

(iii) Orientational polarization.

(iv) Space charge polarization.

(i) Electronic Polarization

The electronic polarization occurs due to the displacement of positive and negative charges in a dielectric material, when an external electric field is applied. The displacement of centre of negatively charged electron cloud relative to the positive nucleus of an atom by

electric field is shown in Fig. 4.15. This shifting of electron cloud results in a dipole moment. Dipole moment is defined as the product of charges and shift distance.

$$p_e = qd \qquad \ldots(4.72)$$

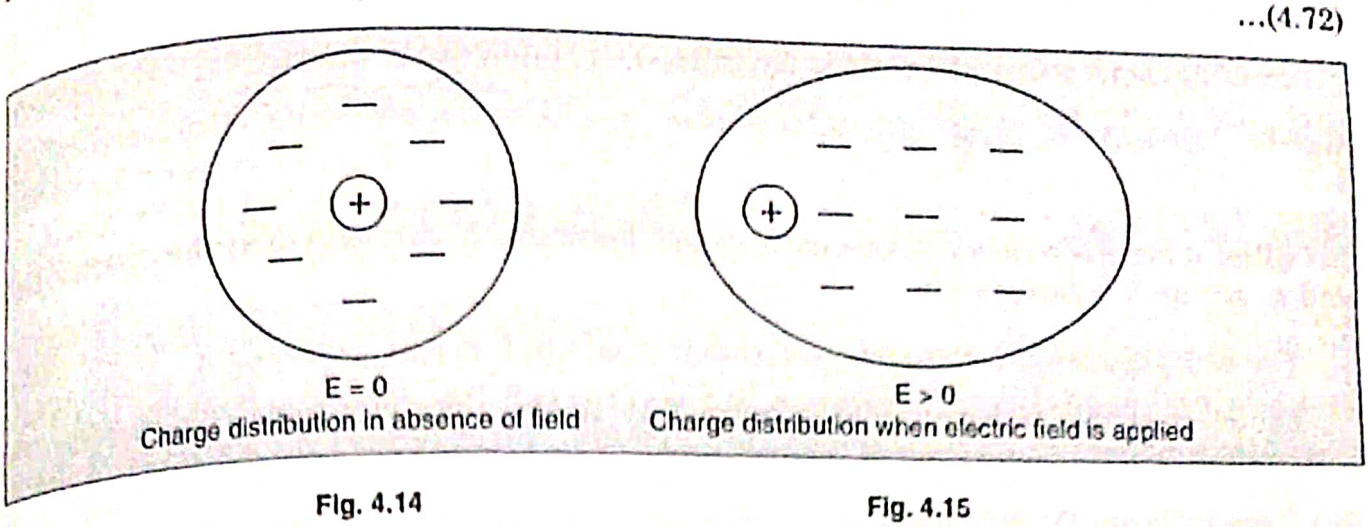


Fig. 4.14 Fig. 4.15

Also the induced dipole moment $(\vec{p})$ is directly proportional to field strength $(\vec{E})$.

$$\vec{p}_e \propto \vec{E} \qquad \ldots(4.73)$$

or

$$\vec{p}_e = \alpha_e \vec{E} \qquad \ldots(4.74)$$

Where α_e is constant of proportionality known as electric polarizability.

If there are n atoms in the dielectric the electronic polarization of the dielectric is given as

$$\vec{P}_e = n\vec{p}_e = n\alpha_e \vec{E} \qquad \ldots(4.75)$$

The electronic polarizability is independent of temperature.

(ii) Ionic Polarization

Ionic polarization occurs only in those dielectric materials which possess ionic bonds such as NaCl. When such a material is subjected to an external electric field, the cations and anions get displaced in opposite directions, which gives rise to a net dipole moment as shown in Fig. 4.16.

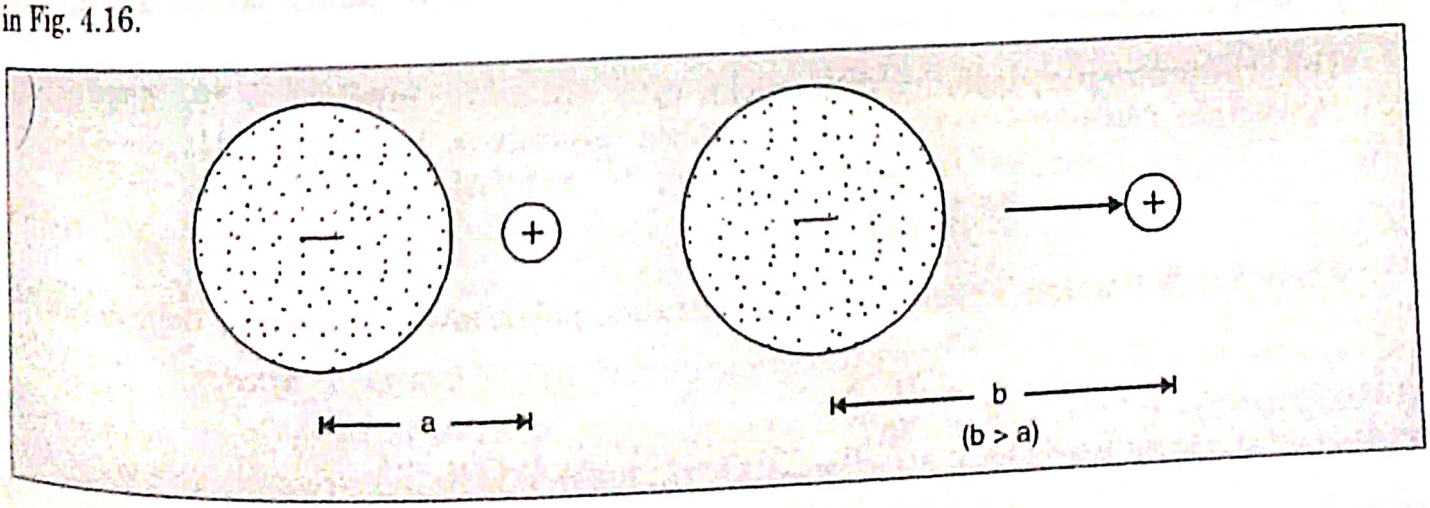


Fig. 4.16

The magnitude of the dipole moment for each ion pair, p_i is equal to product of the relative displacement d_i and charge on each ion i.e.

$$p_i = qd_i \qquad \ldots(4.76)$$

and total ionic polarization of the dielectric

$$\vec{P} = n\alpha_i \vec{E} \qquad \ldots(4.77)$$

where n are the number of ions pairs in the dielectric, $\vec{E}$ strength of applied electric field and α_i the ionic polarizability.

The ions experience electronic polarization in addition to ionic polariation.

For most of the material ionic polarizability is less than electronic polarizability. The polarization is also independent of temperature.

(iii) Orientational Polarization

Polar dielectrics (such as CH_3Cl) exhibits orientational or dipolar polarizability. Even in the absence of external electric field the polar dielectrics exhibits dipole moment. The orientations of molecules are random and hence net dipole moment is zero. The dipole orientations is shown in Fig. 4.17(a).

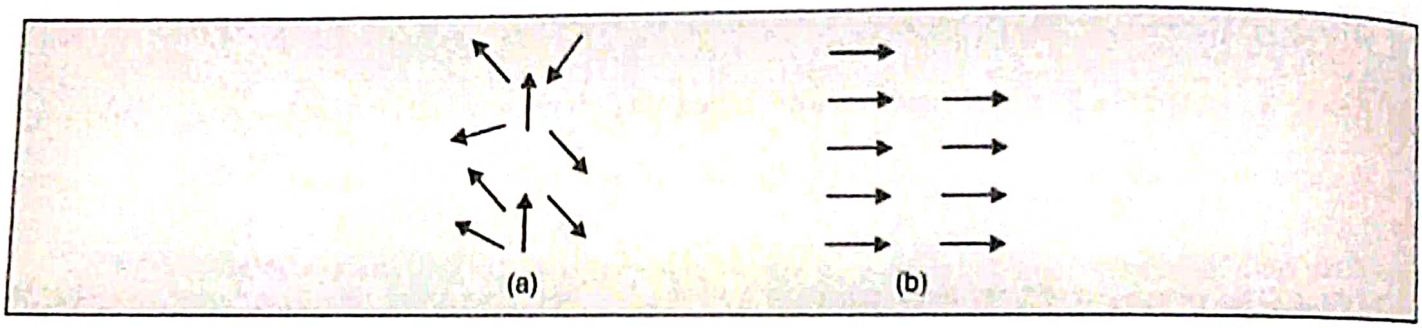


Fig. 4.17

When an external field is applied, the electric field tries to align these dipoles along the direction of field as shown in fig. (4.17b). This type of polarization is known as orientational polarization.

When an external electric field is applied to a polar dielectric, they (dipoles) tends to align themselves in the direction of field. The polarization due to such alignment is called orientation polarization.

The orientation polarizability α_0 is given as

$$\alpha_0 = \frac{p^2}{3kT} \qquad \ldots(4.78)$$

where k is Boltzmann's constant and orientation polarization is given by Debye's Law

$$P_0 = \frac{np^2E}{3kT} \qquad \ldots(4.79)$$

The orientational is strongly temperature dependent and decreases with increase of temperature.

(iv) Space Charge Polarization

This type of polarization occurs due to accumulation of charges at the electrodes or at the interphases in a multiphase material. The ions diffuse over appreciable distances in response to applied field, giving rise to a redistribution of charges in the dielectric medium. This type of polarization is known as **interfacial polarization.**

The total polarization of a material is the sum of electronic, ionic, orientational and space charge polarization

$$P = P_e + P_i + P_o + P_s \qquad \ldots(4.80)$$

4.15 DIELECTRIC STRENGTH

When potential difference between the plates of a capacitor with dielectric in between the plates is increased continuously, the electric field between plates of capacitor will go on increasing and consequently the separation between positive and negative charges of molecules of dielectric will also go on increasing. A stage will reach when the opposite charges of molecule will break off from the molecule and become free. In this situation the dielectric will not remain insulating and behave as a conductor. As a result the capacitor will be discharged.

The **minimum electric field strength applied to the dielectric at which its electric breakdown takes place is called dielectric strength.**

SOLVED PROBLEMS

PROBLEM 1. **A capacitor has capacitance of 100 picofarad. When it is filled with a dielectric its capacitance increases to 250 picofarad. What is the dielectric constant of the dielectric.**

Solution

Given $C_0 = 100\,pF = 100 \times 10^{-12}\,F = 10^{-10}\,F$

$$C = 250\,pF = 250 \times 10^{-12} = 25 \times 10^{-11}\,F$$

$$K = \frac{C}{C_0} = \frac{25 \times 10^{-11}}{10^{-10}} = 2.5$$

PROBLEM 2. **If a sodium chloride crystal is subjected to an electric field of 1000V/m and resulting polarization is 4×10^{-8} cm^{-2}, calculate the relative permittivity of sodium chloride. Given $\epsilon_0 = 8.85 \times 10^{-12}$ Fm^{-1}.**

Solution

Given $\epsilon_0 = 8.85 \times 10^{-12}\,Fm^{-1}$

$$E = 1000\ V/m,\ P = 4 \times 10^{-8}\ cm^{-2}$$

$$P = \epsilon_0 (\epsilon_{r-1}) E \qquad (\epsilon_r = K)$$

$$\text{or} \quad (\epsilon_r - 1) = \frac{P}{\epsilon_0 E}$$

$$\text{or} \quad \epsilon_r = 1 + \frac{P}{\epsilon_0 E} = 1 + \frac{4\times10^{-8}}{(8.85\times10^{-12})\times1000}$$

$$\text{or} \quad \epsilon_r = 1 + \frac{4}{8.85}\times10^{1} = 1 + \frac{40}{8.85}$$

$$\therefore \quad \epsilon_r = 1 + 4.52 = 5.52$$

PROBLEM 3. **The dielectric constant of a medium is 5. Electric field in the dielectric 10^5 *V/m*. Calculate electric displacement and polarization. Take $\epsilon_0 = 9 \times 10^{-12}$ F/m.**

Solution

Given ϵ_r (or K) = 5, $E = 10^5\ V/m$

$$\epsilon_0 = 9\times10^{-12}\ F/m$$

$$\therefore \quad D = \epsilon_0 KE = 9\times10^{-12}\times5\times10^{5} = 45\times10^{-7}\ C/m^2$$

and $$P = \epsilon_0 (K-1)E = 9\times10^{-12}(5-1)\times10^{5}$$

$$= 9\times4\times10^{-7} = 36\times10^{-7}\ C/m^2$$

PROBLEM 4. **An isotropic and homogeneous slab of dielectric constant $K = 4$ and volume 0.5 cm³ is kept normal to an electric field due to which the magnitude of displacement vector is 6×10^{-12} *C/m²*. Calculate (i) the magnitude of electric field (ii) the magnitude of electric polarization and (iii) total induced dipole moment inside the slab.**

Solution

Given $K = 4$, Volume $= 0.5\ \text{cm}^3 = 0.5 \times 10^{-6}\ \text{m}^3$

$$D = 6 \times 10^{-12}\ C/m^2$$

(i) $$D = \epsilon_0 KE$$

$$\text{or} \quad E = \frac{D}{\epsilon_0 K} = \frac{6\times10^{-12}}{(8.86\times10^{-12})\times4} = \frac{6}{8.86\times4}$$

$$= \frac{6}{35.44} = 0.169$$

(ii) $$D = \epsilon_0 E + P$$

$$\text{or} \quad P = D - \epsilon_0 E$$

$$= 6\times10^{-12} - 8.86\times10^{-12}\times0.169$$

$$= (6-1.5)\times10^{-12} = 4.5\times10^{-12}\ C/m^2$$

(iii) Total induced dipole moment

$$= P \times \text{Volume of slab}$$

$$= 4.5 \times 10^{-12} \times 0.5 \times 10^{-6}$$

$$= 2.25 \times 10^{-18}\ \text{C-m}$$

PROBLEM 5. **The dielectric constant of helium is 1.000074. Find the dipole moment of each atom when the gas is subjected to an electric field of intensity 1500 Volt/cm. Given number of atoms per cubic metre is 6.023×10^{23}.**

Solution

Given $E = 1500$ Volt/cm $= 1.5 \times 10^5$ Vm^{-1}

$K = 1.000074$, $n = 6.023 \times 10^{23}$

$$K = 1 + \chi_e = 1 + \frac{P}{\epsilon_0 E}$$

or $$P = \epsilon_0 (K-1) E = 8.85\times10^{-12} \times (1.000074-1)\times1.5\times10^5$$

$$= 8.85\times10^{-12}\times0.000074\times1.5\times10^5$$

$$= 9.82\times10^{-11}\ Cm^{-2}$$

Since $P = p \times n$

or $$p = \frac{P}{n} = \frac{9.82\times10^{-11}}{6.023\times10^{23}}$$

$\therefore$ $p = 1.63 \times 10^{-34}\ C\text{-}m$

PROBLEM 6. **The electric susceptibility of a material is $35.4 \times 10^{-12}\ \frac{C^2}{nt\text{-}m^2}$. What are values of dielectric constant and permittivity of the material ?**

Solution

Given $\chi_e = 35.4\times10^{-12}\ C^2/nt\text{–}m^2$

$$K = 1 + \frac{\chi_e}{\epsilon_0} = 1 + \frac{35.4\times10^{-12}}{8.85\times10^{-12}}$$

$$= 1 + 4 = 5$$

$$\epsilon = \epsilon_0 K = 8.85\times10^{-12}\times5 = 44.3\times10^{-12} C^2/nt - m^2$$

PROBLEM 7. If helium gas consisting of non-polar atoms, has an electric susceptibility $7 \times 10^{-25}\ C^2/nt\text{-}m^2$. Find the dipole moment induced in the atom and atomic polarizability, if the gas is subjected to an electric field of 10^3V/m.

Solution

$$\chi_e = 7\times10^{-25}\ C^2/nt-m^2, E=10^3\ V/m$$

$$P = \epsilon_0\ \chi_e E = 8.85\times10^{-12}\times7\times10^{-25}\times10^3$$

$$= 61.95 \times 10^{-34}\ \text{C/m}^2$$

If number of atoms per unit volume = n

Since one mole of gas at N.T.P. has 6×10^{23} molecules and occupies volume 22.4 litre.

$$\therefore \quad n = \frac{6\times10^{23}}{22.4\times10^{-3}} = 0.268\times10^{26}\ m^{-3}$$

$$np = P$$

$$p = \frac{P}{n} = \frac{61.85\times10^{-34}}{0.268\times10^{26}} = 2.31\times10^{-58}\ \text{C-m}$$

Also $\quad p = \alpha E$

$$\therefore \quad \alpha = \frac{p}{E} = \frac{2.31\times10^{-58}}{10^3} = 2.31\times10^{-61}\ Fm^2$$

PROBLEM 8. Assume that negative charge on hydrogen atom is distributed uniformly over the volume of an atom of radius 0.5A°. The atom is placed in an electric field of 300 V/cm. Find polarizability of the atom.

Solution

Given $\quad R = 0.5\text{A}° = 0.5 \times 10^{-10}\ \text{m} = 5 \times 10^{-11}\ \text{m}$

$$E = 300\ \text{V/cm} = 3 \times 10^4\ \text{Vm}^{-1}$$

$$\alpha = (4\pi\epsilon_0)R^3$$

$$= \frac{1}{(9\times10^9)}\times(5\times10^{-11})^3 = \frac{125}{9}\times10^{-42}$$

$$= 1.39 \times 10^{-41}\ Fm^2$$

PROBLEM 9. A sample of phosphorous is uniformly polarized and polarization produced is 5×10^{-6} C/m². Find the total surface charge developed on an area of 6 m² inclined at an angle 30° with direction of polarization.

Solution

Given $P = 5\times10^{-6}\ C/m^2$, $A = 6\ m^2$, $\theta = 30°$

$$\sigma_p = \vec{P}.\hat{n} = P\cos\theta$$

$$\sigma_p = 5\times10^{-6}\cos 30° = 5\times10^{-6}\times\frac{\sqrt{3}}{2}$$

$$\therefore \quad \sigma_p = 4.33\times10^{-6}\ C/m^2$$

Total surface charge developed on area A

$$q_p = \iint_A \sigma_p\, dS = \iint_A 4.33\times10^{-6}\, dS$$

$$= 4.33\times10^{-6}\times A$$

$$= 4.33\times10^{-6}\times6 = 2.6\times10^{-6}\,C$$

PROBLEM 10. **What is the atomic polarizability of argon ? Its susceptibility at 273 K at 1 atmosphere is 4.35×10^{-4} and n is 2.7×10^{25} atom/m³.**

Solution

Given $\chi_e = 4.35\times10^{-4}$

$$P = n\alpha E = \epsilon_0(\epsilon_{r-1})E$$

$$\therefore \quad \alpha = \frac{\epsilon_0(\epsilon_{r-1})}{n} = \frac{8.85\times10^{-12}\times(4.35\times10^{-4})}{2.7\times10^{25}}$$

$$= \frac{38.4975}{2.7}\times10 = 1.43\times10^{-40}\ Fm^2$$

PROBLEM 11. **The dielectric constant of helium gas at N.T.P. is 1.0000684. Calculate electronic polarizability of the gas containing 2.7×10^{25} atoms/m³.**

Solution

Given $n = 2.7\times10^{25}$ atoms/m³

$$\epsilon_r = 1.0000684$$

$$\alpha_e = \frac{\epsilon_0(\epsilon_{r-1})}{n}$$

$$= \frac{8.85\times10^{-12}\times(1.0000684-1)}{2.7\times10^{25}}$$

$$= \frac{8.85\times10^{-12}\times0.0000684}{2.7\times10^{25}}$$

$$= 2.24 \times 10^{-41}\ Fm^2$$

PROBLEM 12. A solid dielectric, with density 3.5×10^{26} atoms/m^3 shows an electronic polarizability 10^{-38} farad m^2. Assuming the internal electric field to be a Lorenz field, calculate the dielectric constant of the material.

Solution

Given $n = 3.5\times10^{26}$ atoms/m^3

$$\alpha_e = 10^{-38}\ Fm^2$$

$$\epsilon_r = 1+\frac{N\alpha_e}{\epsilon_0}$$

$$= 1+\frac{3.5\times10^{26}\times10^{-38}}{8.85\times10^{-12}}$$

$$= 1+\frac{3.35}{8.85} = 1 + 0.378$$

$$= 1.378$$

CONCEPTUAL QUESTIONS

Q. 1. **What is a dielectric ?**

Ans. A material which does not conduct electricity but on applying electric field the induced charges are produced on its faces is called a dielectric.

Q. 2. **What is dielectric strength of a material ?**

Ans. The maximum value of electric field that dielectric can withstand without electric break down is called dielectric strength of the material.

Q. 3. **Define dielectric constant.**

Ans. It is defined as the ratio of capacitance of a capacitor with dielectric to the capacitance of the capacitor without dielectric

$$K = \frac{C}{C_0}$$

Q. 4. **Discuss importance of dielectrics.**

Ans. Dielectrics are insulators but when placed between the plates of the capacitor, they increase the capacity of the capacitor and also increase the energy stored per unit volume of the capacitor.

Q. 5. Define polarization.

Ans. Polarization is defined as the process of creating or inducing dipoles in a dielectric medium by an external electric field.

Q. 6. What is the difference between free charges and bound charges ?

Ans. Charges on the plates of the capacitor are called free charges, they can move freely on the plates. On the other hand induced charges on opposite sides of a dielectric due to polarization, when placed in an electric field are immobile, hence they are called bound charges.

Q. 7. On what factors polarization of a dielectric depends ?

Ans. Polarization of a dielectric depends upon

(i) Strength of applied electric field and

(ii) Temperature of the dielectric

Q. 8. State the condition under which the alignment of molecules in a polar dielectric is perfect.

Ans. The temperature of the sample should be zero degree Kelvin.

Q. 9. What is atomic polarizability? What are its units ?

Ans. It is defined as the ratio of the induced dipole moment to the applied electric field.

i.e. $$\alpha = \frac{p}{E_0}$$

$$\text{units of } \alpha = \frac{p}{E} = \frac{C-m}{V/m} = \text{farad-metre}^2$$

Q. 10. How dielectric constant K is infinity for metals ?

Ans. We know that

$$K = \frac{\sigma}{\sigma - \sigma_p}$$

where charge density of polarization for metals

$$\sigma_p = \sigma$$

$$\therefore \quad K = \infty \text{ for metal}$$

Q. 11. Is polarization possible in air or vacuum ?

Ans. No, because air possesses no atoms or molecules which can be polarized.

Q. 12. What do you mean by local field ?

Ans. In solids, a molecule or atom experiences not only the external field, but also the field produced by dipoles as well. As a result of the long range coulomb forces, the latter contribution can not be neglected. This resulting field is called local field, and it is responsible for polarizing individual molecules or atoms of solids.

Q. 13. What do you mean by electronic polarization ?

Ans. On placing a dielectric material in an electric field the positive and negative charges of an atom or molecule which are coinciding in the absence of electric field get displaced. This displacement of positive and negative charge is termed as electronic polarization.

Q. 14. What is ionic polarization ?

Ans. When external electric field is applied across an ionic solid, then cations and anions in the molecule move in opposite direction. This type of polarization is called ionic polarization.

Q. 15. What do you understad by orientation polarization ?

Ans. When an external electric field is applied across polar dielectric material, then dipoles of the material experience torque and start rotating so as to align themselves in the direction of external electric field. This is called orientation polarization.

Q. 16. Name different types of polarization.

Ans. Following are different types of polarization

(i) Electronic Polarization

(ii) Ionic Polarization

(iii) Orientation Polarization

(iv) Space Charge Polarization

Net polarization vector

$$\vec{P} = \vec{P}_e + \vec{P}_e + \vec{P}_o + \vec{P}_s$$

Q. 17. What is the significance of electric susceptibility for a dielectric ?

Ans. We know that susceptibility of a dielectric is given by

$$\chi = \frac{P}{\epsilon_0 E_0}$$

This equation shows that χ is large for a dielectric if P is large, hence it represents that how easily a dielectric can be polarized.

Q. 18. Explain dielectric loss.

Ans. It is the loss of electric energy in the form heat by a dielectric material during polarization process when subjected to an a.c. voltage.

Q. 19. What is the relationship between dielectric constant k and electric susceptibility χ_e?

Ans. $K = 1 + \chi_e$

Q. 20. Derive the relation $\vec{D}, \vec{E}$ and $\vec{P}$.

Ans. We know that

$$E = E_0 - E_p$$

Or $$E_0 = E + E_p$$

$$\frac{\sigma_f}{\epsilon_0} = E + Ep \qquad \left(\because E_0 = \frac{\sigma_f}{\epsilon_0}\right)$$

or $$\sigma_f = \epsilon_0 E + \epsilon_0 E_p$$

or $$\sigma_f = \epsilon_0 E + \epsilon_0 \left(\frac{\sigma_p}{\epsilon_0}\right) \qquad \left(\because E_p = \frac{\sigma_p}{\epsilon_0}\right)$$

or $$\sigma_f = \epsilon_0 E + \sigma_p$$

Since $$D = \sigma_f \text{ and } P = \sigma_p$$

$\therefore$ $$D = \epsilon_0 E + P$$

In vector form

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P}$$

MULTIPLE CHOICE QUESTIONS

1. **Which of the following substances are dielectric (s) ?**

   (a) copper (b) mica

   (c) germcnium (d) tungsten

2. **The centres of gravity of positive and negative charges coincides in**

   (a) H_2 (b) HCl

   (c) CO (d) H_2O

3. **The relation between three electric vectors $\vec{E}, \vec{D}$ and $\vec{P}$**

   (a) $\vec{D} = \vec{P} + \vec{E}$ (b) $\vec{D} = \frac{\vec{P}}{\vec{E}}$

   (c) $\vec{D} = \epsilon_0 \vec{E} + \vec{P}$ (d) $\vec{D} = \epsilon_0 (\vec{E} + \vec{P})$

4. **The relation between dielectric constant k and dimensionless, electric susceptibility χ_e is**

   (a) $K = 1 + \epsilon_0 \chi_e$ (b) $K = 1 - \chi_e$

   (c) $K = 1 + \chi_e$ (d) $K = \epsilon_0 \chi_e$

5. **The unit of ϵ_0 is**

(a) Cm^{-2} (b) Fm^{-1}

(c) Dimensionless (d) Hm^{-1}

6. **The unit of relative dielectric constant is**

(a) Cm^{-2} (b) Fm^{-1}

(c) Dimensionless (d) CV^{-1}

7. **In $\vec{D} = \epsilon_0 \vec{E} + \vec{P}, \vec{P}$ is connected with**

(a) Free charges only (b) Bound charges only

(c) Free and bound charges both (d) None of these

8. **In general, the effect of temperature on relative permittivity of a material is to**

(a) reduce it (b) increase it

(c) maintain it (d) All of the above

9. **Which of the following mechanism is/are temperature dependent :**

(a) Electronic polarization (b) Ionic polarization

(c) Both (a) and (b) (d) Orientation polarization

10. **Which of the following polarization arises due to alignment of random molecules**

(a) Electronic (b) Ionic

(c) Orientation (d) Space charge

11. **The electronic polarization α_e of a monoatomic gas atom is**

(a) $4\pi\epsilon_0$ (b) $4\pi \epsilon_0 R$

(c) $4\pi \epsilon_0 R^3$ (d) $4\pi \epsilon_0 R^2$

12. **Ionic polarization**

(a) Decreases with temperature (b) Increases with temperature

(c) May increase or decrease with temperature (d) Is independent of temperature

13. **With increase in temperature, the orientation polarization in general**

(a) Increases

(b) Decreases

(c) Is constant

(d) First increases then becomes constant

14. **The dielectric constant of an insulator may be**

(a) –1 (b) 0

(c) 0.3 (d) 3

15. **Which of the following is non-zero for vacuum ?**

(a) Conductivity of heat (b) Conductivity of electricity

(c) Permittivity (d) None of these

16. **Clausius-Mossitti equation is a relation between**

(a) polarizability and dielectric constant

(b) paramagnetic and diamagnetic

(c) electronic and ionic polarizability

(d) permeability and susceptibility.

17. **Which of the following is not a component of polarizability**

(a) volume polarizability (b) space charge polarizability

(c) orientational polarizability (d) ionic polarizability

18. **Out of all four known polarization mechanisms which requires maximum electrostatic energy to be supplied is**

(a) space charge polarization (b) ionic polarization

(c) orientational polarization (d) electronic polarization

19. **Dielectric medium should have property**

(a) high dielectric constnat (b) high specific resistance

(c) high dielectric strength (d) all

20. **Electronic polarizability of an atom is proportional to**

(a) radius (b) $(\text{radius})^2$

(c) $(\text{radius})^3$ (d) $\sqrt{\text{radius}}$

21. **Choose the correct relation for orientation polarizability**

(a) $\alpha_0 = p^2 kT$ (b) $\alpha_0 = \dfrac{p^2}{kT}$

(c) $\dfrac{3kT}{p^2}$ (d) $\alpha_0 = \dfrac{p^2}{3kT}$

22. **The electric field which a dipole experiences in a medium is**

(a) called the local field (b) called the internal field

(c) (a) and (b) (d) equal to external field

23. **Expression for internal field (Lorentz field) is given by**

(a) $E_i = E - \dfrac{P}{3\epsilon_0}$ (b) $E_i = E + \dfrac{3P}{\epsilon_0}$

(c) $E_i = E - \dfrac{3P}{\epsilon_0}$ (d) $E_i = E + \dfrac{P}{3\epsilon_0}$

24. Clausius-Mossotti equation with usual meaning of notations can be written as

(a) $\alpha_e = \frac{1}{N}\left(\frac{\epsilon_r + 2}{\epsilon_r - 1}\right)$ (b) $\alpha_e = \frac{3\epsilon_0}{N}\left(\frac{\epsilon_r + 1}{\epsilon_r - 1}\right)$

(c) $\alpha_e = \frac{3\epsilon_0}{N}\left(\frac{\epsilon_r - 1}{\epsilon_r + 2}\right)$ (d) $\alpha_e = \frac{N\epsilon_0}{3}\left(\frac{\epsilon_r + 2}{\epsilon_r - 1}\right)$

Answers

1.	(b)	2.	(a)	3.	(c)	4.	(c)	5.	(b)
6.	(c)	7.	(b)	8.	(d)	9.	(d)	10	(c)
11.	(c)	12.	(d)	13.	(b)	14.	(d)	15.	(c)
16.	(a)	17.	(a)	18.	(d)	19.	(d)	20.	(c)
21.	(d)	22.	(c)	23.	(d)	24.	(c)		

CHAPTER AT A GLANCE

1. Dielectrics are insulators. They possess high electrical resistivity. When a dielectric is placed in an external electric field, induced charges are produced on its opposite faces. Examples : Glass, Mica, Wax, Water, Air etc.

2. Dielectric constant of a material is defined as the ratio of the capacitance of a capacitor with dielectric to the capacitance of the capacitor without dielectric (i.e. air as medium).

$$K = \frac{C}{C_0} \text{ also } K = \frac{\sigma_f}{\sigma_f - \sigma_p}$$

3. Classification of dielectrics. Dielectrics are of two types.

(i) Polar dielectrics. The dielectrics whose each molecule possesses permanent electric dipole moment. The centre of gravity of positive and negative charges of these molecules do not coincide. In the absence of electric field, these molecules are randomly oriented and the resultant electric dipole moment of the dielectric sample is zero. But on applying external electric field, they try to align in the direction applied field. Such dielectrics are called polar dielectrics.

(ii) Non-polar dielectrics. The dielectric is said to be non-polar if dipole moment of each molecule of the sample is zero in the absence of external electric field. When electric field is applied, the molecules of the dielectric sample becomes induced electric dipole.

4. Polarization of dielectric. The process of creating or inducing dipoles in a dielectric medium by an external electric field is called polarization. Polariation of a dielectric depends upon (i) strength of applied electric field and (ii) temperature of the dielectric.

5. Polarization Vector ($\vec{P}$). The induced dipole moment per unit volume of a dielectric

is called polarization vector $\vec{P}$. Polarization vector of a dielectric is numerically equal to surface charge density of bound charges.

$$P = \sigma_p$$

6. Susceptibility. Polarization density is directly proportional to the product of net electric field $\vec{E}$ inside the dielectric and electric permeability of free space (ϵ_0)

$$\vec{P} \propto \epsilon_0 \vec{E} \text{ or } \vec{P} = \epsilon_0 \chi_e \vec{E}$$

$$\chi_e = \frac{P}{\epsilon_0 E} \text{ called electric susceptibility}$$

7. Relation between K and χ_e

$$K = 1 + \chi_e$$

8. Relation between $\vec{E}, \vec{P}$ and $\vec{D}$

(i) $\vec{D} = \epsilon_0 \vec{E} + \vec{P}$

(ii) $\vec{D} = \epsilon \vec{E}$

(iii) $\vec{P} = \epsilon_0 (K - 1) \vec{E}$

9. Atomic polarizability. It is defined as the ratio of the induced dipole moment to the applied electric field

$$\alpha = \frac{p}{\epsilon_0}$$

Units of α are farad-metre^2

10. Non-uniform polarization of dielectric

In case of non uniform polarization of dielectric

$$\vec{\nabla} . \vec{P} = -\rho_p$$

11. Local field at an atom

In solids, an atom (or molecule) experiences not only the external electric field, but also field produced by dipoles as well. As a result of the long range coulomb forces, the latter contribution can not be neglected. This resulting field is called local field and it is responsible for polarizing individual atoms or molecules of solids. Local electric field is given by

$$E_{loc} = E + \frac{P}{3\epsilon_0}$$

This is known as Lorentz relation

12. Clausius-Mossotti equation

$$\alpha = \frac{3\epsilon_0}{n}\left(\frac{\epsilon_r - 1}{\epsilon_r + 2}\right)$$

13. Types of polarization. Following are difference types of polarization

(i) Electronic polarization

(ii) Ionic polarization

(iii) Orientation polarization

(iv) Space charge polarization.

14. Dielectric strength. The maximum value of electric field that a dielectric can withstand without electric break down is called dielectric strength of the material.

SHORT ANSWER QUESTIONS

1. What is a dielectric ? Give two examples of dielectric.
2. Define dielectric constant of a material.
3. Define dielectric strength.
4. What do you mean by dielectric strength ?
5. What do you mean by polar and non-polar molecules ? Give two examples each.
6. What are polar and non-polar dielectrics ?
7. Define the terms dipole moment and polarization.
8. What do you mean by polarization of a dielectric ?
9. Define two electric vectors $\vec{D}$ and $\vec{E}$. What is the relation between them ?
10. Define electric polarization vector $\vec{P}$. What is its S.I. units?
11. Explain the term permittivity.
12. What do you understand by electric displacement, susceptibility and permittivity ?
13. What is dielectric polarization and electric displacement vector?
14. Establish the relation

$$D = \epsilon_0 E + P$$

Where ϵ_0 is permittivity of vacuum.

15. Name mechanism of dielectric polarization.
16. Derive the relation between dielectric constant and suscepitibility.
17. Define atomic polarizability.

18. Name different types of polarization.
19. Explain that electric field inside the dielectric is reduced when it is placed inside the electric field.
20. What do you understand by local field at an atom ?
21. What is local field at an atom ?

LONG ANSWER QUESTIONS

1. What is dielectrics ? Define dielectric constant of a material.
2. Explain the phenomenon of dielectric polarization in dielectric materials. Define dielectric constant.
3. Explain the terms atomic polarizability, diectric susceptibility and atomic dipole moment.
4. Prove that $K = 1 + \chi_e$, where K is dielectric constant and χ_e is electric susceptibility.
5. What is the effect of introducing a dielectric between the plates of a capacitor. Hence establish the relation $K = 1 + \chi_e$, where letters have their usual meaning.
6. Define atomic polarizability α. Show that the dipole moment in an atom subjected to field $\vec{E}_0$, is given by $\vec{p} = \alpha \vec{E}_0$.
7. Define polarizability. Give its S.I. units. Establish the relation between polarizability and dielectric constant.
8. A dielectric acquires a polarization $\vec{P}$ in an electric field $\vec{E}$. Show that it acquires :

   (i) Volume change density $\rho_p = -\vec{\nabla}.\vec{P}$ and

   (ii) Surface charge density $\sigma_p = \vec{P}.\vec{n}$.
9. Derive an expression for atomic polarizability of an atom.
10. Show that for non uniform polarization.

$$\vec{\nabla}.\vec{P} = -\rho_p$$

11. Derive the relation $\vec{D} = \epsilon_0 \vec{E} + \vec{P}$.
12. Define and explain the three vectors $\vec{P}$, $\vec{E}$ and $\vec{D}$. Why electric field inside a dielectric decreases due to polarization ? Show that $\vec{D} = \epsilon_0 \vec{E} + \vec{P}$. Also give their units.

13. Show that the electric field inside a polarized dielectric due to induced polarization charge is $\vec{E}_p = -\frac{\vec{P}}{\epsilon_0}$ where $\vec{P}$ is polarization density vector.

14. Define local field at an atom. Derive the relation between local field and polarization of a dielectric.

15. Derive Clausius-Mossotti relation between polarizability and dielectric constant of a solid.

16. Derive Clausius-Mossotti relation.

17. Derive molecular interpretation of Clausius-Mossotti equation.

18. Deduce the Clausius-Mossotti relation for polarization of a medium and explain how it could be used to determine dipole moment of polar molecules.

19. Explain classical Theory of electronic polarizability.

20. Discuss different types of polarization. Discuss the frequency dependence of these polarizations.

21. Define polar and non-polar molecules. Deduce Clausius Mossotti relation for non-polar dielectrics.

UNSOLVED NUMERICAL PROBLEMS

1. A capacitor has the capacitance of 50 pF. Its capacity increse to 400 pF when it is filled with dielectric. Calculate the value of dielectric constant of dielectric.

[Ans. 8]

[Hints. $K = \frac{C}{C_0} = \frac{400 \times 10^{-12}}{50 \times 10^{-12}} = 8$]

2. If a NaCl crystal is subjected to an electric field of 2000 V/m and the resulting polarization is 4.3×10^{-8} C/m^2, calculate relative permittivity of NaCl.

[Ans. 3.43]

[Hints. $\epsilon_r = 1 + \frac{P}{\epsilon_0 E} = 1 + \frac{4.8 \times 10^{-8}}{8.85 \times 10^{-12} \times 2000} = 3.43$]

3. Calculate the electronic polarizability of argon atom. Given $\epsilon_r = 1.0024$ at N.T.P and $N = 2.7 \times 10^{25}$ atoms/m^3.

[Ans. $7.9 \times 10^{-40}\ Fm^2$]

[Hints. $\alpha_e = \frac{\epsilon_0(\epsilon_{r-1})}{N} = \frac{8.85\times10^{-12}(1.0024-1)}{2.7\times10^{25}} = 7.9\times10^{-40}\ Fm^2$]

4. The dielectric constant of argon at 0°C and at one atomosphere is 1.000435. Calculate polarizability of the atom. [Ans. $1.43 \times 10^{-40}\ Fm^2$]

[Hints. $\alpha_e = \frac{\epsilon_0(\epsilon_{r-1})}{N}, \epsilon_r = 1.000435, \epsilon_0 = 8.85\times10^{-12}$ F/m $N = \frac{6\times10^{26}}{22.4} = 2.6\times10^{25}$]

5. The electric field in a sample of polystyrene at 25°C is uniform with a magnitude of 5000 V/m. Find (i) The polarization in polystyrene (ii) Electric displacement vector. Given the dielectric constant of polystyrene at 25°C is 2.56 and $\epsilon_0 = 8.85 \times 10^{-12}$ $C^2N^{-1}\ m^2$. [Ans. (i) $6.9\times10^{-8}\ C/m^2$; (ii) $1.33 \times 10^{-7}\ C/m^2$]

[Hints. $\chi_e = \epsilon_{r-1} = 2.56-1 = 1.56$, $P = \epsilon_0 \chi_e E = 8.85\times10^{-12}\times1.56\times5000 = 6.9\times10^{-8}$
$D = \epsilon_0 E + P = 8.85 \times 10^{-12} \times 5000 + 6.9 \times 10^{-8} = 1.33 \times 10^{-7}\ C/m^2$]

6. The electric field in a sample of sulphur having dielectric constant 3.48 is measured to be 50V/m. Find (a) polarization in the sulphur (b) electric displacement.

[Ans. (a) $1.1\times10^{-9}\frac{C}{m^2}$ (b) $1.5\times10^{-9}\frac{C}{m}$]

[Hints. $\chi_e = \epsilon_{r-1} = 3.48-1 = 2.48$, $P = \epsilon_0 \chi_e E = 8.85\times10^{-12}\times2.48\times50 = 1.1\times10^{-9}\ C/m^2$
$D = \epsilon_0\epsilon_r E = 8.85\times10^{-12}\times3.48\times50 = 1.5\times10^{-9}\frac{C}{m}$]

7. A solid elemental dielectric has a density of 3×10^{28} atoms/m^3 shows an electronic polarizability of $10^{-40}\ Fm^2$, Assuming Lorentz field, calculate dielectric constant of the material. [Ans. 1.34]

[Hints. $\epsilon_r = 1 + \frac{N\alpha_e}{\epsilon_0} = 1 + \frac{3\times10^{28}\times10^{-40}}{8.85\times10^{-12}} = 1.34$]

8. A sample of phosphorous is uniformly polarized and polarization produced 5×10^{-8} C/m^2. Find the total surface charge developed on an area $5m^2$ inclined at an angle of 60° with direction of polarization. [Ans. 1.25×10^{-7} C]

[Hints. $\sigma_p = \vec{P}.\vec{n} = P\cos\theta = 5\times10^{-8} \times \cos 60° = 5\times10^{-8}\times\frac{1}{2} = 2.5\times10^{-8}\ C/m^2$

$q_p = \iint_A \sigma_p dS = \iint_A 2.5\times10^{-8} dS = 2.5\times10^{-8}\times5 = 1.25\times10^{-7}\ C$]

9. Show that when polarization of a medium is uniform, polarization vector is solenoidal.

[**Hints.** For a non uniform polarization $\vec{\nabla}.\vec{P}=-\rho_p$. For uniform polarization $\vec{\nabla}.\vec{P}=0$. Hence polarization for such a distribution is solenoidal.]

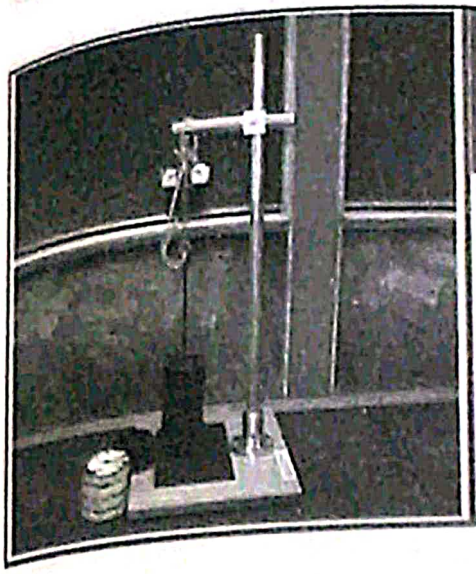
10. An electric field of 9×10^4 V/m is applied on a sample of neon gas at N.T.P. Calculate the dipole moment induced in each atom, if the dielectric constant of neon at N.T.P. is 1.000134. Find the atomic polarizability of neon.

[**Ans.** 3.92×10^{-36} C-m, 0.435×10^{-40} $\frac{C-m^2}{\text{Volt}}$]

[**Hints.** $p=\frac{P}{n}=\frac{\epsilon_0(\epsilon_r-1)E}{n}=\frac{8.85\times10^{-12}\times(1.000134-1)\times9\times10^4\times22.4}{6.023\times10^{26}}=3.92\times10^{-36}$ C-m.

$\alpha_e=\frac{p}{E}=\frac{3.92\times10^{-36}}{9\times10^4}=0.435\times10^{-40}\ C\text{-}m^2/\text{Volt}$]

□□□



Chapter 5

LASERS

Laser in one of the important device developed in the past half century. It is an optical amplifier that produces highly directional, monochromatic and coherent light. The word laser stands for light amplification by stimulated emission of radiation. Einstein in 1917 predicted the phenomenon of stimulated emission caused by light radiation of proper frequency. The laser works on this phenomenon of stimulated emission. In 1954 C.H. Towns developed a microwave amplifier called maser. The word maser stands for microwave amplification by stimulated emission of radiation. The first laser device was developed in 1960 by T.H. Maiman. It is called Ruby laser. The laser is often referred as optical maser because it operates in the visible portion of e.m. spectrum. Ruby laser emits red light of wavelength 694 nm. Now laser action has been obtained with ions, atoms and molecules in gases, liquids, solids and semiconductors, in the range from ultraviolet to radio frequency region. Today laser find wide use in communication, computers, navigation, holography, biology, medicine, military warfare, long distance measurement etc.

5.1 CHARACTERISTICS OF LASER LIGHT

Light from a laser differs from light of convential sources in number of ways. The most striking features of laser beam are :

(i) Directionality

(ii) High intensity

(iii) High degree of coherence and

(iv) Etraordinary monochromaticity

(i) Directionality. An ordinary light source emits light waves in all the directions in the form of spherical waves and are highly divergent Apertures are used to produce narrow beams of light from such sources. But laser emits radiations only in one direction. The divergence or angular spread of a laser radiations (light) is very small. **The directionality of laser beam is usually expressed in terms of full angle beam divergence which is twice the angle that the outer edge of the beam makes with the axis of the beam. The outer edge of the beam is a point at which the strength of the beam falls to 1/e times its value at the centre.**

The beam of light with plane wavefront coming from an aperture of diameter d,

propagates as a parallel beam for a distance $\frac{d^2}{\lambda}$ which is called **Rayleigh range** as shown in Fig. 5.1.

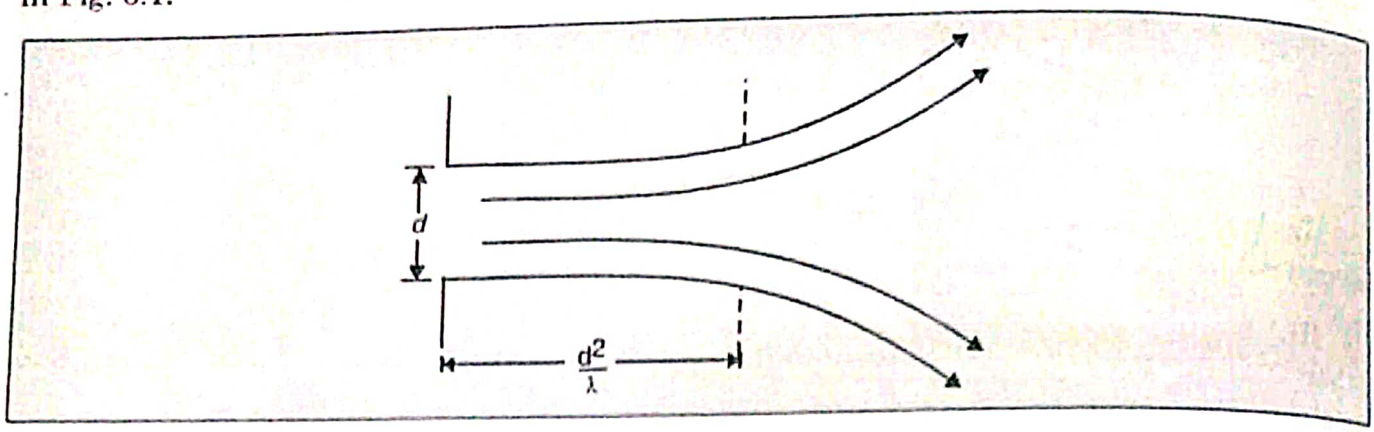


Fig. 5.1

It then begins to spread because of diffraction. The angular spread of the beam is given by

$$\Delta 0 = \frac{\lambda}{d} \qquad ...(5.1)$$

where λ is wavelength of laser light and d is diameter of aperture. In a typical laser, the beam divergence is less than 0.1 milliradian. For gas lasers, the angular divergence can be as low as 10^{-5} radians. Thus laser beam is highly directional.

(ii) High Intensity. Light from a lamp comes out almost uniformly in all directions. At a distance of 30 cm from a 100 watt filament lamp, power entering the eye is less than 10^{-3} watt. Laser beam is highly intense and can be focussed at a point i.e. at a small area. These radiation form a highly directional collimated beam with only a very small angle of divergence. On the other hand, conventional light sources emit radiations in all directions. For laser beam divergence is about 1 milliradian or 0.0057 degree. Taking into account the diffraction effects, a laser beam can be focussed to a region of radius about $\frac{\lambda f}{a}$, where λ is wavelength of light, f local length of lens and 'a' is radius of lens or laser beam.

For a lens of $a = 0.05\ m$, $f = 0.1\ m$ and $\lambda = 5 \times 10^{-7}\ m$

$$\text{Area of spot of light} = \pi\left(\frac{\lambda f}{a}\right)^2$$

$$= 3.14 \times \left(\frac{5 \times 10^{-7} \times 0.1}{0.05}\right)^2$$

$$= 3 \times 10^{-12}\ m^2$$

Intensity of light is defined as the energy passing normally per unit area per second through a point normal to the direction of flow. For an ordinary spherical source, at a distance r, the intensity is given by

$$I = \frac{P}{4\pi r^2} \quad \ldots(5.2)$$

where P is power of the source.

For a 1 watt laser, the intensity of light in the plane of lens is given by

$$I = \frac{P}{A} = \frac{1}{3\times10^{-12}} = 3.3\times10^{11}\ Wm^{-2}$$

In case of laser beam, the energy is concentrated in a very small region. 1 watt laser source will be many times more intense than ordinary 100 watt source.

(iii) High degree of coherence. The main characteristic which distinguishes laser from other sources is coherence. Coherence is the measure of degree of phase. Correlation that exists in the radiation field of light. Laser radiations has characteristic of high degree of coherence. The other characteristics of laser (i.e. directionality, intensity, monochromaticity) are in one way or the other related to coherence. The coherence is of two types

(I) Spatial Coherence and

(II) Temporal Coherence

(I) Spatial Coherence

Spatial coherence is also known as **"transverse coherence." A beam of light is said to possess spatial coherence if the phase difference of the waves crossing two points on a plane perpendicular to the direction of propagation of beam is time independent.**

Hence, if there is no phase difference between two points or phase difference between them is zero, then the two waves are in spatial coherence. For this reason, spatial coherence is called transverse coherence.

Consider a beam of light travelling along X-axis. Let *ABCD* is a plane perpendicular to beam (or X-axis). Let P and Q are two points on this plane within the beam of light as shown in Fig. 5.2.

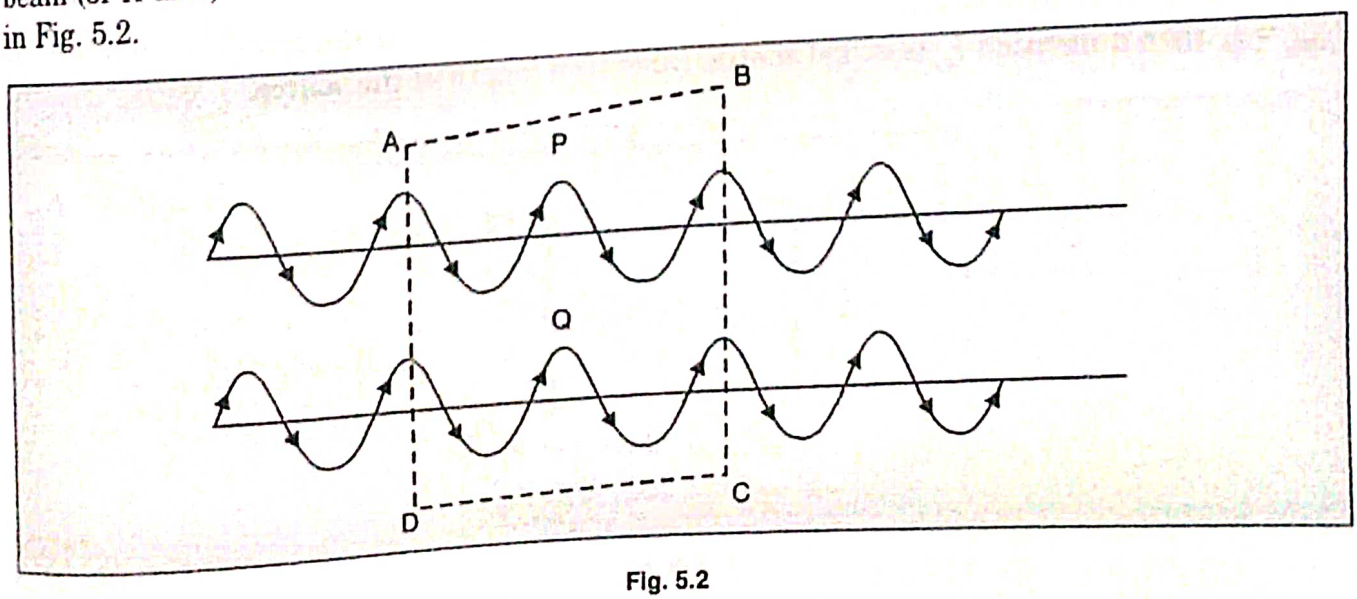


Fig. 5.2

Let phase of waves crossing points P and Q at any instant be ϕ_P and ϕ_Q, then phase difference of waves crossing points P and Q is given by

$$\Delta\phi = \phi_P - \phi_Q \qquad \ldots(5.3)$$

If $\Delta\phi$ is independent of time (or always constant) then beam of light is said to possess spatial coherence.

Let us explain spatial coherence due to a point source S as shown in Fig. 5.3.

Point Source. Let A and B are two points lying on the line joining them with source S. The phase relationship between A and B depends the distance AB.

If $AB << L$

Where L is coherence length, there will diffi a definite phase relationship between points A and B and there will be a high coherence between A and B. On the other hand if

$$AB >> L$$

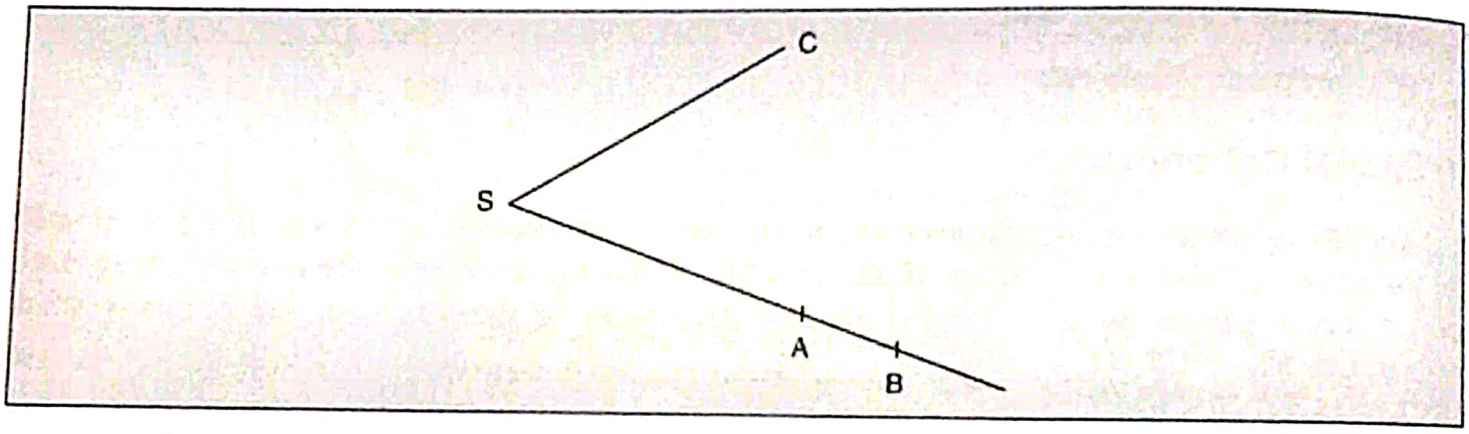


Fig. 5.3

There will be no coherence between A and B. Now if we consider points A and C which are equidistant from point source S, then waves will reach points A and C exactly in the same phase, hence the two points will have perfect spatial coherence.

In Fig. (5.4) S_1 and S_2 are two slits separated by distance l. If the interference occurs for $l_{max} = l_s$ then dimension l_s is called spatial coherence length of the source.

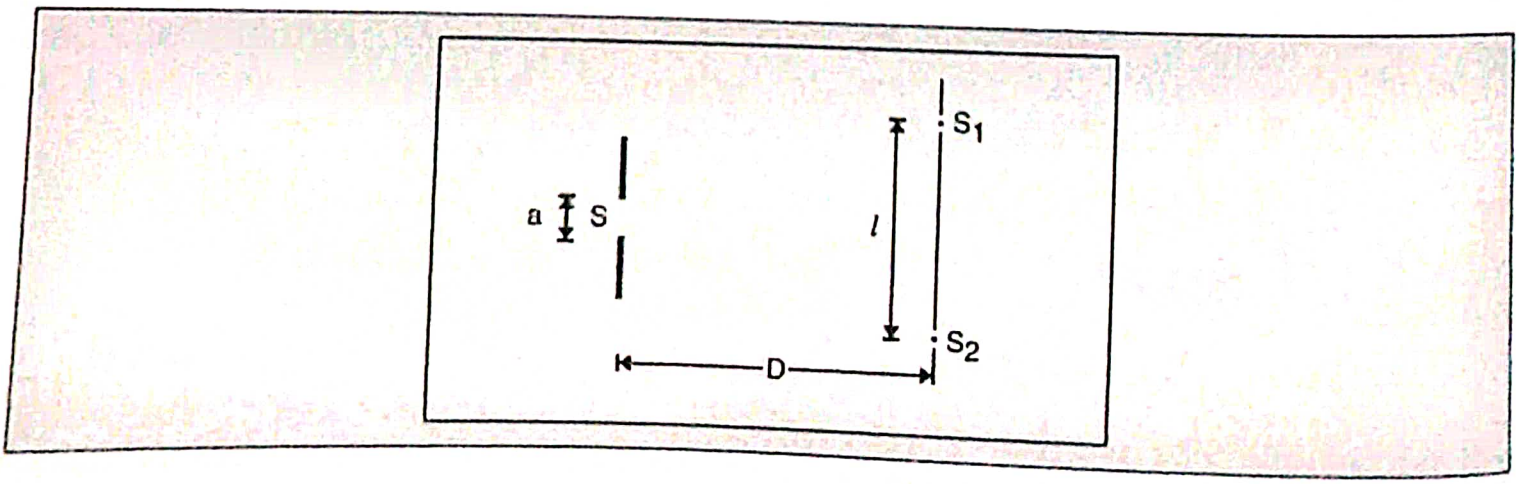


Fig. 5.4

The source S is at a distance D from slits S_1 and S_2. The condition for coherence of S_1 and S_2 is

$$\frac{\lambda}{a} > \frac{l}{D}$$

or

$$l < \frac{\lambda}{a/D}$$

Since $\frac{a}{D} = \theta$, angle subtended by slit S. Thus

$$l_s = \frac{\lambda}{\theta} \qquad \ldots(5.4)$$

II. Temporal Coherence. Temporal coherence is also known as longitudinal coherence. **Temporal coherence is a measure of relation between the phases of a wave at different points along the direction of propagation of wave.**

Consider a light wave travelling along X-axis as shown in Fig. (5.5). Let A and B are two points on the wave, which lie on X-axis. Let ϕ_A and ϕ_B are the phases of wave at points A and B at any time. Then, phase difference between these points

$$\Delta\phi = \phi_A - \phi_B \qquad \ldots(5,5)$$

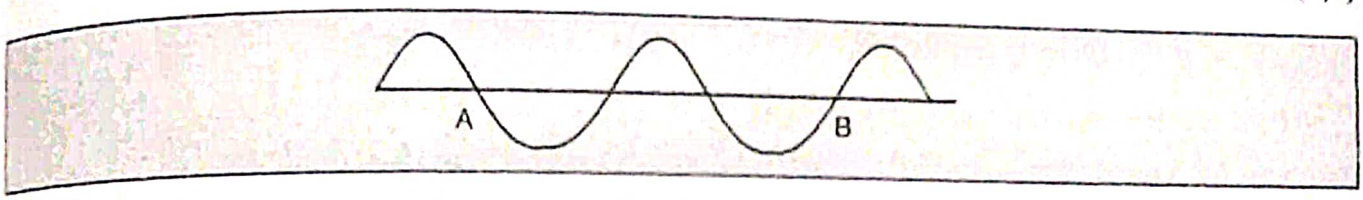


Fig. 5.5

If $\Delta\phi$ is independent of time, then wave is said to have temporal coherence.

Thus if the phase difference of the wave crossing two points lying along the direction of propagation of wave is independent of time (i.e. phase difference is constant), then wave is said to have temporal coherence.

The average time-interval for which the field remains sinusoidal (i.e. definite phase relationship exists) is called coherence time T_c. The corresponding distance L is called coherence length.

$$L = T_c \times c \qquad \ldots(5.6)$$

where c is velocity of light

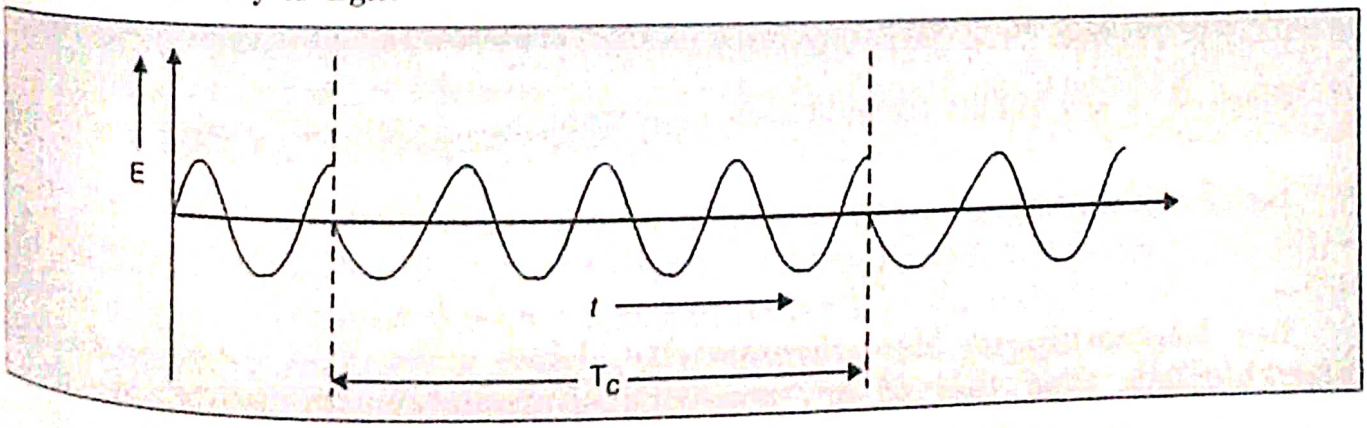


Fig. 5.6

$\therefore$ Coherence length = Coherence time × velocity of light.

In considering characteristics of light, we assumed that the wave produced by source is always sine wave. This is not true. In fact, there is a slow and random variation of frequency with time around central frequency as shown in Fig. (5.6).

Coherence time (T_c) is of the order of reciprocal of frequency range ($\Delta\nu$)

$$T_c = \frac{1}{\Delta\nu} \qquad \ldots(5.7)$$

Putting this value in eq. (5.6), we get

$$L = cT_c = \frac{c}{\Delta\nu}$$

Or $$L = \frac{c}{\Delta\nu} \qquad \ldots(5.8)$$

Since $$\nu = \frac{c}{\lambda}$$ where λ is wavelength of light

$\therefore$ $$\Delta\nu = -\frac{c}{\lambda^2}\Delta\lambda$$

Putting this value in eq. (5.8), we get

$$L = -\frac{c\lambda^2}{c\Delta\lambda}$$

Or $$L = -\frac{\lambda^2}{\Delta\lambda}$$

Neglecting negative sign

$$L = \frac{\lambda^2}{\Delta\lambda}$$

Or $$\Delta\lambda = \frac{\lambda^2}{L} \qquad \ldots(5.9)$$

This is known as line width.

Since $\frac{\lambda}{\Delta\lambda} = Q$ is quality factor of each wave train.

Hence coherence length in terms of quality factor can be written as

$$L = \lambda Q \qquad \ldots(5.10)$$

(iv) Extraordinary Monochromaticity. Laser emits light which is much more monochromatic than that of any conventional monochromatic source. In case of a conventional monochromatic source light with one frequency is never possible and it is

spread over a frequency range (i.e. band of frequencies) around a central frequency. This band of frequencies $\Delta\nu$ is called **line width or band width.**

The light from conventional sources has band width of the order of 10^{10} Hz or more where as band width in case of laser is of the order of 100 Hz. The degree of monochromacity of a wave may be defined as its relative band width given by

$$\text{Monochromacity} = \frac{\Delta\nu}{\nu_0} \qquad \ldots(5.11)$$

where ν_0 is the central frequency of the light.

If ν_0 is zero, then absolute monochromaticcity can be achieved which is not possible. The laser light is however has a high degree of monochromaticity of the order of 10^{-12}.

5.2 STIMULATED ABSORPTION

When the atom in ground state absorbs energy by any means, the electrons of the atom absorbs energy and are excited to higher energy state (excited state).

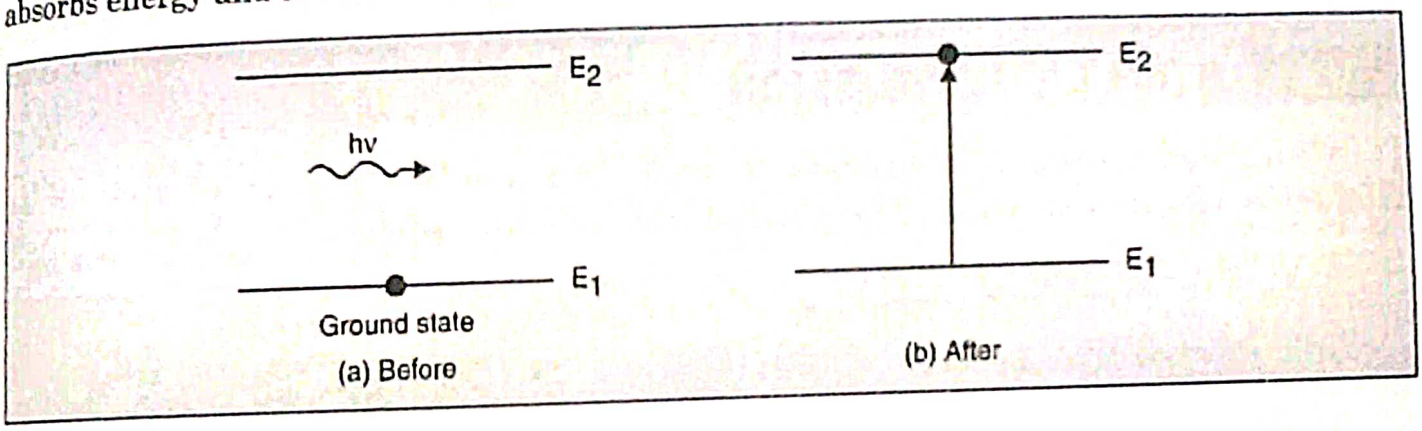


Fig. 5.7

When an atom in the ground state with energy E_1 absorbs a photon of incident radiation, it gets excited to the higher energy state E_2. Then energy absorbed is given by

$$h\nu = E_2 - E_1 \qquad \ldots(5.12)$$

where $h\nu$ is the energy of incident photon. This process is known as stimulated asbortpion or simply absorption as shown in Fig. (5.7). An atom remains in the excited state for a short time 10^{-8} sec and then comes back in the ground state. The average time for which an atom remains in the excited state is called its mean life. Energy state having mean life more than 10^{-8} sec. is called meta-stable state.

5.3 SPONTANEOUS EMISSION

Spontaneous emission takes place when an atom is already in a excited state. No external radiation is required to start the emission process. The excited atom does not remain in the excited state for a long time, it de-excite from excited state E_2 to ground state E_1 by emitting a photon of energy.

$$h\nu = E_2 - E_1 \qquad ..(5.13)$$

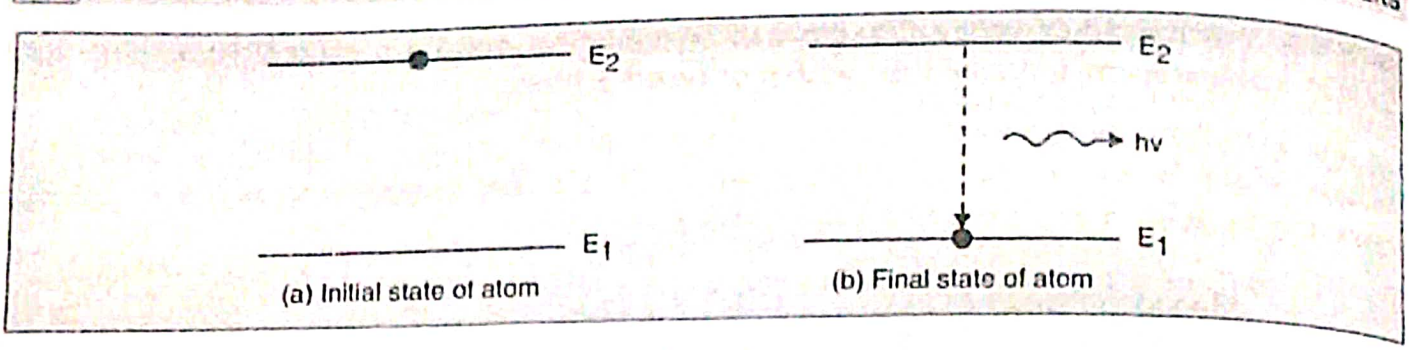


Fig. 5.8

This type of emission is called **spontaneous emission** as shown in Fig. (5.8). If there is an assembly of atoms, the radiation emitted spontaneously by each atom has a radom direction and random phase, incoherent and a broad spectrum. The probability of occurrence of spontaneous emission from state 2 to state 1 is determined by the properties of states 2 and 1. This is denoted as

$$(P_{21})_{\text{spontaneous}} = A_{21} \qquad \ldots(5.14)$$

which is known as **"Einstein's coefficient of spontaneous emission of radiation."**

5.4 STIMULATED EMISSION

Stimulated emission is process in which an incident photon of appropriate frequency triggers an atom in an excited state to emit radiation.

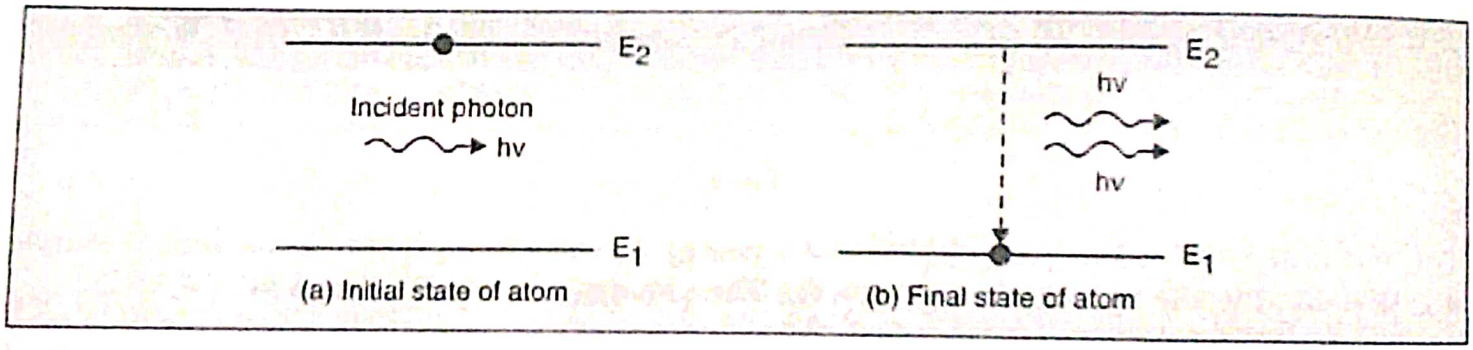


Fig. 5.9

When an atom in an excited state E_2 interacts with a photon of appropriate frequency ν and is stimulated (or induced) to go to ground state E_1 it emits the difference of energy $E_2 - E_1$ in the form of a photon of the same frequency ν as shown in Fig. (5.9). The emitted photon travels in the same direction as that of incident photon i.e. the two photons are in phase with each other. The direction of propagation, phase, energy and state of polarization of the emitted photon is exactly the same as that of the incident stimulating photon, so the result is an enhanced beam of coherent light.

The probability of stimulated emission transition from state 2 to state 1 is proportional to the energy density $u(\nu)$ of stimulating radiation and is given by

$$(P_{21})_{\text{stimulated}} = B_{21}\, u(\nu) \qquad \ldots(5.15)$$

where B_{21} is Einsteins coefficient

5.5 DIFFERENCE BETWEEN SPONTANEOUS EMISSION AND STIMULATED EMISSION

S.No.	Spontaneous Emission	Stimulated Emission
1.	The emission of light photon takes place immediately during transition of atom from higher energy level to lower energy level.	Emission of light photon takes place by inducement of a photon having energy equal to the energy of emitted photon.
2.	The emission has a broad spectrum (i.e. many wavelengths)	The emission has monochromatic radiation.
3.	Incoherent radiation.	Coherent radiation.
4.	Less intense.	Highly intense.
5.	Less directionality and angular spread during propagation	High directionality and less angular spread during propagation.
6.	Example : Light from a sodium lamp or mercury vapour lamp.	Example : Light from a laser source.

5.6 EINSTEIN'S A AND B COEFFICIENTS

Atomic system is characterized by discrete energy states. Atoms usually exists in the lowest energy state (i.e. ground state) Atoms in the lowest energy states may be excited to higher energy by absorbing e.m. radiations (photons) of proper frequency by process called stimulated absorption (or simply absorption). Similarly an atom in the excited state make transaction to a lower energy state by emitting e.m. radiation in two different ways.

(i) The first process is called spontaneous emission in which atom in the excited state emits radiation even in the absence of any incident radiation. The rate of spontaneous emission is proportional to the number of atoms in the excited state (E_2).

(ii) The second process is called stimulated emission, in which incident radiation of proper frequency, triggers an atom in the excited state to emit radiation. The rate of stimulated emission depends on the intensity of the external field as well as the number of atoms in the excited state as shown in Fig. (5.10).

Let E_1 and E_2 are the energies of an atom in the energy states 1 and 2 respectively.

Let N_1 and N_2 be number of atoms per unit volume corresponding to the energy states E_1 and E_2 at any instant.

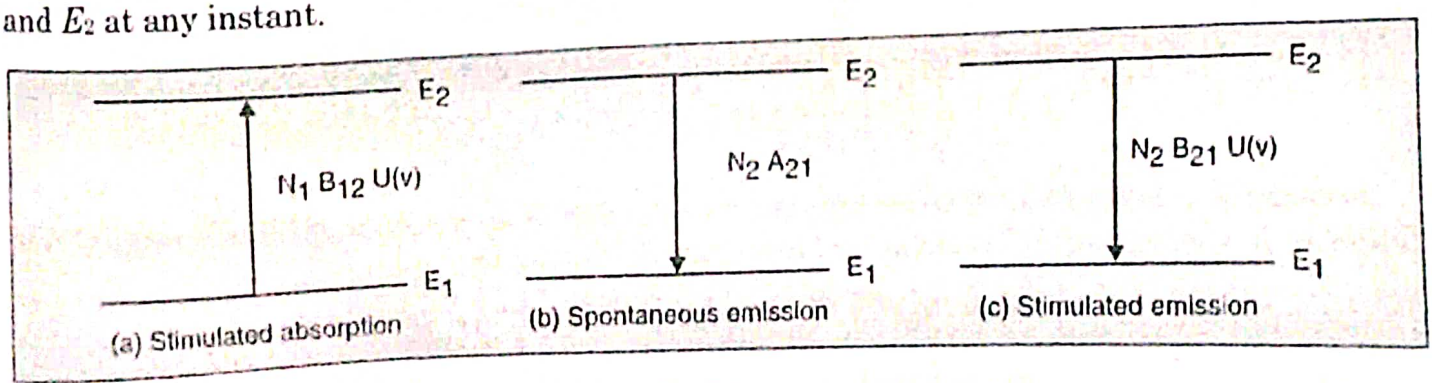


Fig. 5.10

Let $u(\nu)$ is the energy density per unit frequency of the beam of incident photon.

Let photon energy hν is exactly equal to energy difference $(E_2 - E_1)$

$$h\nu = E_2 - E_1$$

Then this photon can excite an atom from state E_1 to E_2.

The rate of absorption would be proportional to N_1 and $u(\nu)$.

The number of absorptions per unit volume per unit time = $N_1 B_{12} u(\nu)$ ...(5.16)

Where B_{12} is a constant of proportionality called Einstein's coefficient of stimulated absorption. For a given value of N_1 and $u(\nu)$, if B_{12} is large then rate of stimulated absorption per unit volume per unit time will also be large. Thus B_{12} represents the probability of absorption of radiation by a substance.

Since the spontaneous emission does not depend on $u(\nu)$. Therefore number of spontaneous emission per unit volume per unit time = $N_2 A_{21}$ ...(5.17)

Where A_{21} is a constant of proportionality called Einstein's coefficient of spontaneous emission. It represents the probability of spontaneous de-excitation by a substance.

Since stimulated emission depends on $u(\nu)$, therefore number of stimulated emission per unit volume per unit time = $N_2 B_{21} u(\nu)$ ...(5.18)

Where B_{21} is a constant of proportionality called Einstein's coefficient of stimulated emission.

At thermal equilibrium rate of absorption is equal to rate of emission. Thus

$$N_1 B_{12} u(\nu) = N_2 A_{21} + N_2 B_{21} u(\nu) \quad \text{...(5.18)}$$

Or $$N_1 B_{12} u(\nu) - N_2 B_{21} u(\nu) = N_2 A_{21}$$

Or $$u(\nu)(N_1 B_{12} - N_2 B_{21}) = N_2 A_{21}$$

Or $$u(\nu) = \frac{N_2 A_{21}}{(N_1 B_{12} - N_2 B_{21})}$$

Or $$u(\nu) = \frac{A_{21}}{\left(\frac{N_1}{N_2}\right) B_{12} - B_{21}} \quad \text{...(5.19)}$$

Where A_{21}, B_{12} and B_{21} are Eintein's coefficients.

$$\therefore \quad u(\nu) = \frac{\frac{A_{21}}{B_{21}}}{\left(\frac{N_1}{N_2}\right)\left(\frac{B_{12}}{B_{21}}\right) - 1} \quad \text{...(5.20)}$$

According to Boltzmann distribution law the number of atoms N_1 and N_2 in energy states E_1 and E_2 in thermal equilibrium at termperature T is given by

$$N_1 = N_0 e^{-E_1/kT}$$

and $$N_2 = N_0 e^{-E_2/kT}$$

where N_0 is the total number of atoms present in the ground state and k is Boltzmann's constant

$$\therefore \quad \frac{N_2}{N_1} = \frac{N_0 e^{-E_2/kT}}{N_0 e^{-E_1/kT}}$$

$$\text{or} \quad \frac{N_2}{N_1} = \frac{e^{-E_2/kT}}{e^{-E_1/kT}}$$

$$\text{or} \quad \frac{N_2}{N_1} = e^{-(E_2-E_1)/kT}$$

But $E_2 - E_1 = h\nu$

$$\therefore \quad \frac{N_2}{N_1} = e^{-h\nu/kT}$$

$$\text{or} \quad \frac{N_1}{N_2} = e^{h\nu/kT}$$

Putting this value in eq. (5.20), we get

$$u(\nu) = \frac{\frac{A_{21}}{B_{21}}}{\frac{B_{12}}{B_{21}} e^{h\nu/kT} - 1} \qquad \ldots(5.21)$$

The Planck's radiation formula of energy density at a given temperature is

$$u(\nu) = \frac{8\pi h\nu^3}{c^3} \frac{1}{e^{h\nu/kT} - 1} \qquad \ldots(5.22)$$

Comparing equations (5.21) and (5.22), we get

$$\frac{A_{21}}{B_{21}} = \frac{8\pi h\nu^3}{c^3} \qquad \ldots(5.23)$$

$$\text{or} \quad \frac{A_{21}}{B_{21}} \propto \nu^3 \qquad \ldots(5.24)$$

$$\text{and} \quad \frac{B_{12}}{B_{21}} = 1 \qquad \ldots(5.25)$$

$$\text{or} \quad B_{12} = B_{21}$$

Equations (5.23), (5.24) and (5.25) are known as Einstein relations

From eq. (5.24)

$$\frac{A_{21}}{B_{21}} \propto \nu^3$$

i.e. the ratio of Einstein's coefficients of spontaneous emission and stimulated emission is proportional to ν^3. It means the probability of spontaneous emission dominates over stimulated emission more and more with increase in energy difference of two states.

5.7 POPULATION INVERSION AND METASTABLE STATES

For laster action to take place the stimulated emission should predominate over spontaneous emission. This is possible only if the number of atoms in the excited state is more as compared to number of atoms in the ground state.

According to Boltzman's Equation

$$N_2 = N_1 e^{-(E_2 - E_1)/kT} \qquad \ldots(5.26)$$

where N_1 and N_2 are the number of atoms in the lower energy state E_1 and higher energy state E_2 respectively.

As $E_2 > E_1$ therefore $N_2 < N_1$

The process of achieving greater population density of atoms in the higher energy state as compared to the lower energy state is called population inversion. The atoms from lower energy states are raised to higher energy states by use of external energy.

Ordinarily, an atom remains in an excited state for about 10^{-8} sec, after which it emits a photon and drops to lower energy state. The emission of photons from an excited atom is governed by well established selection rules. These rules do not permit certain transitions from higher energy level to ground state. Such energy levels are termed as metastable. Once the valence electron find itself in the metastable state, it continues to be there for long time (about 10^{-3} sec.) and the atom is unable to return to the ground state instantaneously. The existence of metastable state is an essential requirement for obtaining population inversion.

To explain the population inversion, consider atoms the given sample of matter are irradiated by radiations of given frequency ν, which results in stimulated absorption of photons raising the electron from ground state E_0 to energy level E_2 as shown in Fig. (5.11a). Suppose in between E_0 and E_2 there is an energy level E_1 which is metastable state. The atom may drop to ground state by spontaneously emitting the photon of the same energy as absorbed by it or it may drop to metastable state E_1 by emitting a photon of energy $E_2 - E_1$. This transition can also occur by non-radiative process. Since E_1 is the metastable state the atom will continue in this state for a long time. As time goes on, more and more atoms will

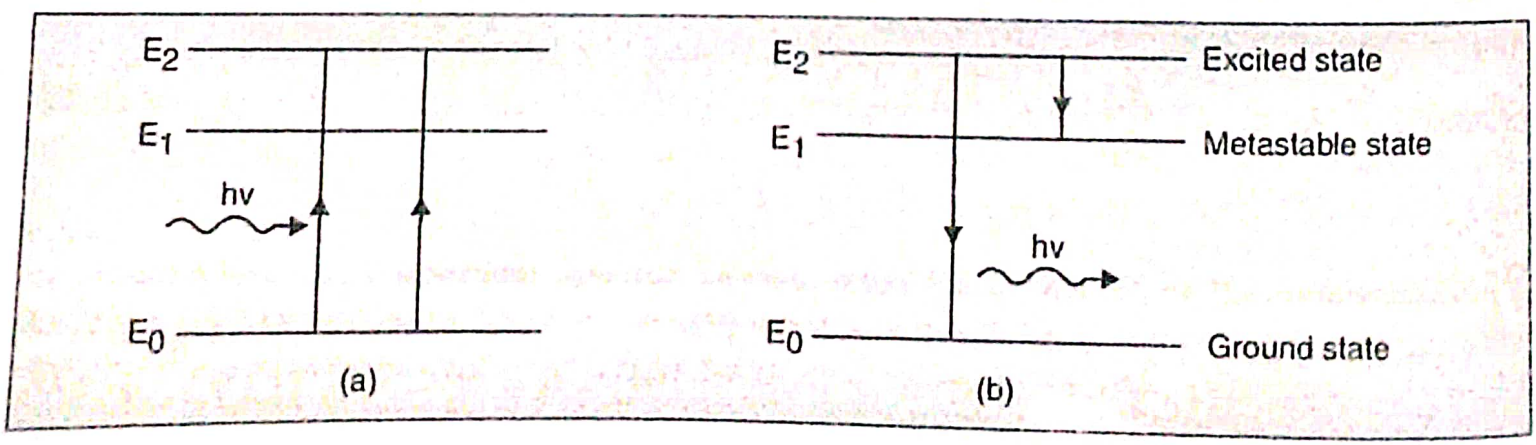


Fig. (5.11)

come in the metastable state E_1 and ultimately the numbers of atoms in state E_1 may be more than in ground state E_0 as shown in Fig. (5.11b). Thus population inversion can be obtained.

5.8 PUMPING

The process of exciting laser medium with suitable form of external energy in order to achieve population inversion is called pumping. The external device used is called a pump. The type of pumping depends upon the type of laser system. There are several ways of pumping a laser.

The most commonly used methods of pumping are the following :

(1) Optical Pumping, (2) Electric Discharge Pumping, (3) Direct Conversion, (4) Chemical Reactions, (5) Inelastic Atom-Atom Collisions.

In the following table different types of pumping used for different types of laser systems are given .

S.No.	Name of Laser System	Type of Pumping
1.	CO_2 Laser	Chemical Reaction
2	Ruby Laser (3 level)	Optical Pumping
3	Gaseous Ion Laser	Electric Discharge
4	Semiconductor Laser (2 level)	Direct Conversion
5	Helium Neon Laser (4 level)	Electric Discharge

In optical pumping the light source which supplies energy is used. The xenon flash lamp is most commonly used optical source.

In case of CO_2 laser, it is chemical reaction between hydrogen and fluorine which provides energy for pumping.

$$H_2 + F_2 \rightarrow 2HF + \text{Energy} \qquad \ldots(5.27)$$

5.9 VARIOUS LEVEL LASER SYSTEMS

(i) Two Level Laser System

If only two energy levels are involved in the laser action, the laser system is known as two level laser system as shown in Fig. (5.12)

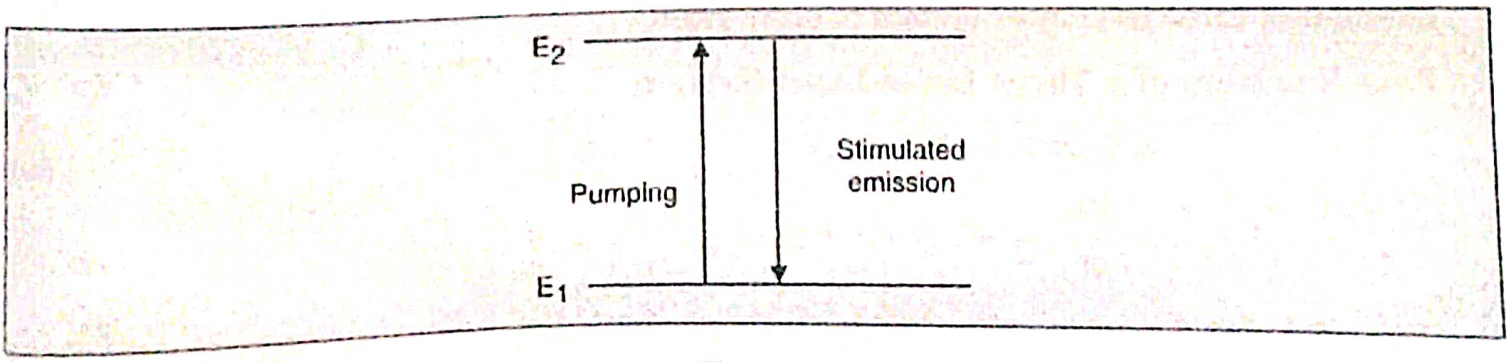


Fig. 5.12

For two level laser system

$$\text{Quantum Efficiency } (\eta) = \frac{E_2 - E_1}{E_2 - E_1} = 1 \qquad \ldots(5.28)$$

i.e. $\eta = 100\%$

Example of two laser system is **Semiconductor Laser System** i.e. light emitting p-n junction diode. In this case laser action occurs between conduction band and valence band.

(ii) Three Level Laser System

If three levels are involved in the laser action, the laser system is known as three level laser system.

In three level system a shown in Fig. (5.13), the atoms are pumped from energy level E_1 to E_3, for example with xenon flash lamp, a large number of atoms are excited through stimulated absorption from energy level E_1 to E_3. The life time of atoms in the energy level E_3 is very short i.e. E_3 is an unstable state. The atoms make transitions from level E_3 to E_2 level. The energy level E_2 is the matastable state and has relatively longer life time as compared to E_3, hence atoms tend to accumulate at E_2. With intense pumping from E_1 to E_3 and because of rapid decay to energy level E_2, the population of atoms becomes move in energy state E_2 as compared to energy state E_1. The stimulated emission occurs between energy level E_2 to energy level E_1 producing laser light.

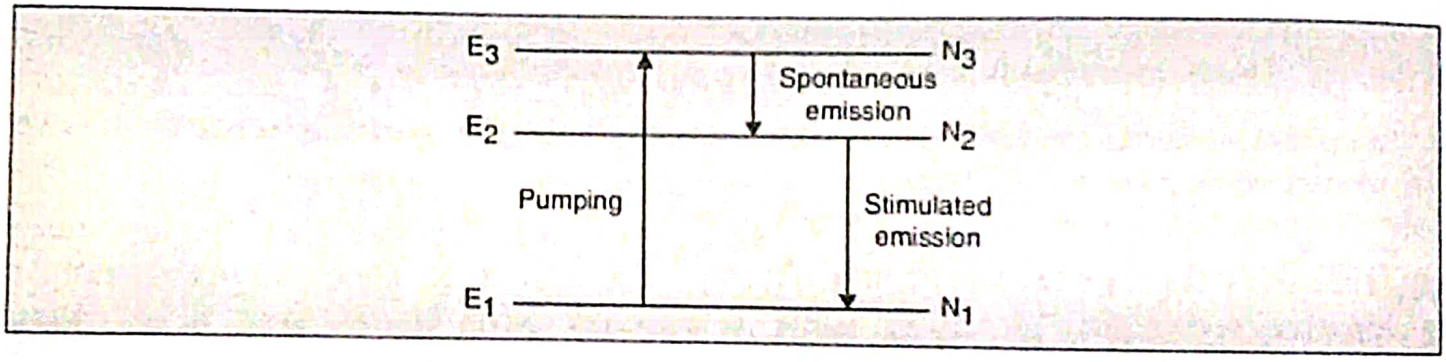


Fig. 5.13

Quantum efficiency (η) of three level laser system is given as the ratio of output energy (i.e. E_2–E_1) to the input energy (i.e. E_3–E_1)

$$\text{Quantum efficiency } (\eta) = \frac{E_2 - E_1}{E_3 - E_1} < 1 \qquad \ldots(5.29)$$

Example of three level laser system is Ruby laser.

Rate Equation of a Three Level-Laser System

$$dN_2/dt = B_{12}N_1I - A_{21}N_2 \qquad \ldots(5.30)$$

$$\frac{dN_1}{dt} = -B_{12}N_1I + A_{21}N_2 \qquad \ldots(5.31)$$

Where B-coefficient term refers to absorption and A-coefficient term refers to stimulated emission and I is pump intensity.

If total number of atoms = N

Then $N \approx N_1 + N_2$

And $\Delta N \approx N_1 - N_2$

Or $2N_2 \approx N_1 - \Delta N + N_2$

$\approx N_1 - (N_1 - N_2) + N_2$

$\approx (N_1 + N_2) - (N_1 - N_2)$

or $2N_2 \approx N - \Delta N$

and $2N_1 \approx N + \Delta N$

Let us $B_{12} = B_{21} = B$

and $A_{21} = A$

Subtracting eq. (5.30) from eq. (5.31), we get

$$\frac{d}{dt}(N_1 - N_2) = -2BIN_1 + 2AN_2$$

or $$\frac{d}{dt}(\Delta N) = -2BIN_1 + 2AN_2$$

$$= -BI(2N_1) + A(2N_2)$$

$$= -BI(N + \Delta N) + A(N - \Delta N)$$

or $$\frac{d}{dt}(\Delta N) = -BIN - BI\Delta N + AN - A\Delta N \quad \ldots(5.32)$$

The inversion is possible in steady in a three level laser system if

Or $0 = -BIN - BI\Delta N + AN - A\Delta N$

$$A\Delta N + BI\Delta N = AN - BIN$$

or $$(A + BI)\Delta N = (A - BI)N$$

or $$\Delta N = \frac{(A - BI)N}{(A + BI)}$$

or $$\Delta N = \frac{\left(\frac{A}{A} - \frac{B}{A}I\right)N}{\left(\frac{A}{A} + \frac{B}{A}I\right)}$$

or $$\Delta N = \frac{\left(1 - \frac{I}{I_{sat}}\right)N}{\left(1 + \frac{I}{I_{sat}}\right)} \quad \ldots(5.33)$$

where $I_{sat} = \frac{A}{B}$ is saturation intensity

Hence if $I > I_{sat}$ ΔN is negative

(iii) Four Level Laser System

In four level laser system four energy levels are involved in the laser action.

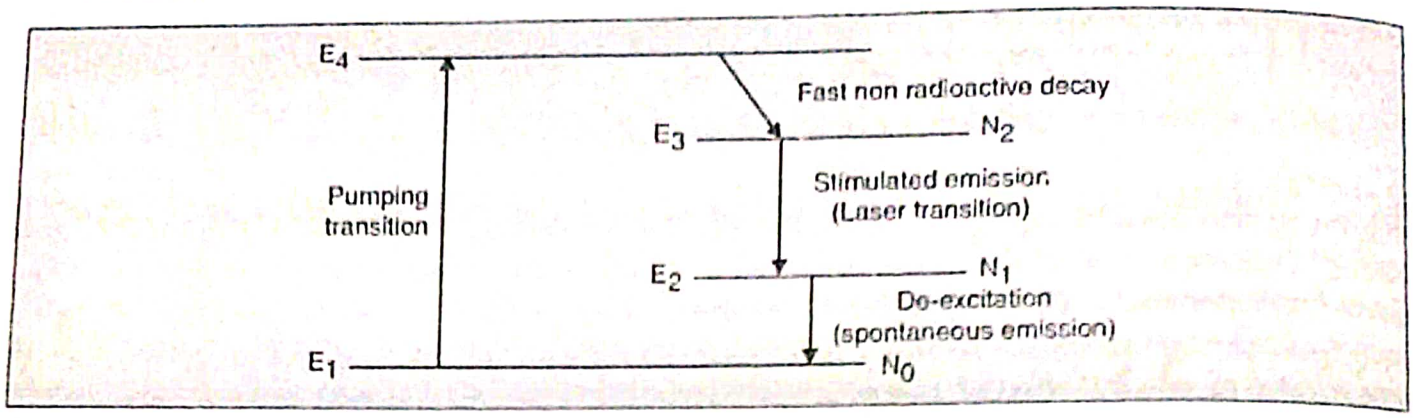


Fig. 5.14

In four level scheme as shown in Fig. (5.14), the atoms from ground state E_1 are raised to the excited state E_4 by pumping. From this energy state E_4 the atoms decay to energy state E_3 by spontaneous non radiative transition. The life time of atoms in the excited state is of the order of 10^{-8} sec. The energy state E_3 is a metastable state. The transition rate of atoms from energy state E_4 to E_3 is much faster as compared to transition from energy state E_3 to E_2 (i.e. 10^{-6} sec.). So the number of atoms in the energy state E_3 exceeds the number of atoms in energy state E_2. Thus population inversion is build up between E_3 and E_2. The laser action takes place between E_3 and E_2 by stimulated emission. The population inversion on E_3 to E_2 transition in four level laser system can be achieved and maintained with moderate pumping. Since in this scheme level E_2 in the lower laser level (not ground level) it relatively easier to maintain population inversion between levels E_3 and E_2 with moderate pumping and get continuous wave output. For this to happen the transition from energy state E_2 to E_1 must be very fast. The atoms from energy state E_2 simply get de-excited from energy state E_2 to ground state E_1.

He-Ne laser is an example of a four level laser.

In this case energy given to laser medium by pumping per excitation is given as

Input energy = $E_4 - E_1$

Energy given out by laser per lasing de-excitation energy is given as

Output energy = $E_3 - E_2$

$$\therefore \text{Quantum efficiency} = \frac{\text{Output energy}}{\text{Input energy}}$$

$$\eta = \frac{E_3 - E_2}{E_4 - E_1} \qquad \ldots(5.34)$$

It is clear from the schemes of both three and four level systems that the quantum efficiency of a three level laser is more than corresponding four level laser. However, the quality of three level laser beam is expected to be poor as compared to four level laser.

Rate Equations for a Four Level Laser System

Assume the lower level 1 rapidly decays to ground level 0 as shown in Fig. (1.15).

Let N_o, N_1 and N_2 are number of atoms is the ground state (0), level 1 and level 2 respectively. We can write.

$$\frac{dN_2}{dt} = B_{12}\, NoI - A_{21}\, N_2 \qquad \ldots(3.35)$$

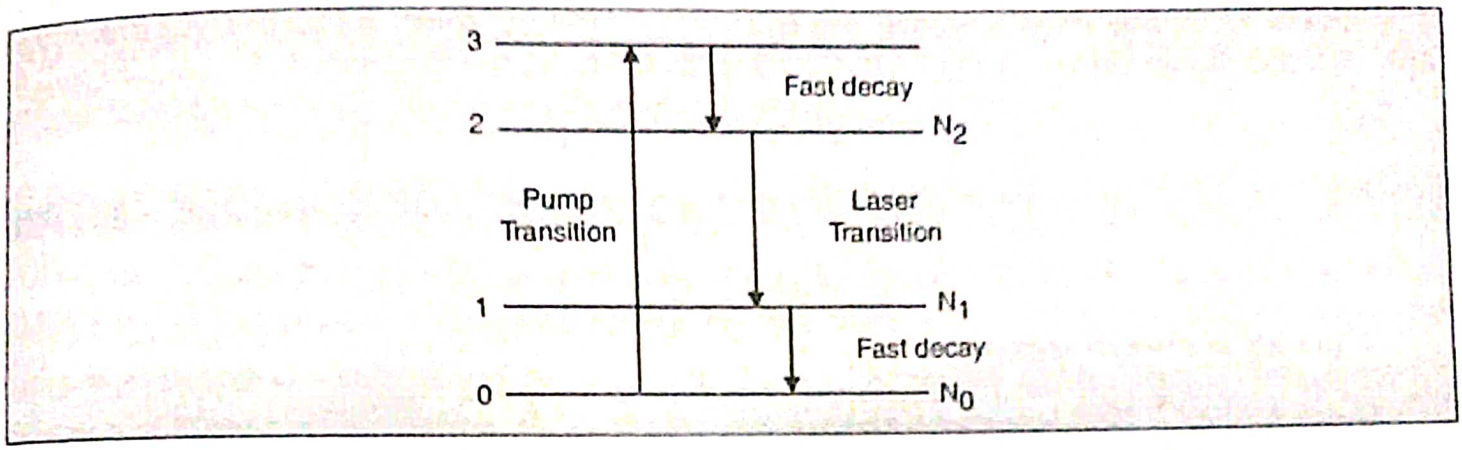


Fig. 1.15

Where B-coefficient term refers to absorption and A-coefficient term refers to stimulated emission and I is pump intensity.

Here total number of molecules is

$$N \approx N_o + N_2$$

Or $$No \approx N - N_2$$

Putting this value in eq. (3.35), we get

$$\frac{dN_2}{dt} = B_{12}\,(N - N_2)\, I - A_{21}\, N_2 \qquad \ldots(3.36)$$

Since $$N_1 = 0$$

$$\Delta N = -N_2$$

Write B for B_{12} and A for A_{12} in eq. (3.36), we get

$$\frac{-d(\Delta N)}{dt} = B\,(N - N_2)\, I - A\, N_2$$

or $$\frac{-d(\Delta N)}{dt} = B(N + \Delta N)I + A\Delta N$$

or $$\frac{-d(\Delta N)}{dt} = BIN + BI\Delta N + A\Delta N \qquad \ldots(3.37)$$

At steady state $\frac{d(\Delta N)}{dt} = 0$

$\therefore$ Eq. (3.37) becomes

or $$0 = BIN + BI\Delta N + A\Delta N$$

$$(A + BI)\Delta N = -BIN$$

or $$\Delta N = -\frac{BIN}{(A+BI)}$$

or $$\Delta N = -\frac{\frac{B}{A}IN}{\left(\frac{A}{A}+\frac{B}{A}I\right)}$$

or $$\Delta N = -N\frac{\left(\frac{I}{I_{sat}}\right)}{\left(1+\frac{I}{I_{sat}}\right)} \quad \ldots(3.38)$$

Thus ΔN is always negative

Here $I_{sat} = \frac{A}{B}$ is saturation intensity.

Where A is the excited relaxation rate $\left(\frac{1}{\tau}\right)$ and B is absorption cross section divided by the energy per photon i.e. $\sigma/h\nu$. Both depends upon the molecules, the frequency and various states involved.

$\therefore$ $$I_{sat} = \frac{h\nu}{\sigma\tau} \quad \ldots(3.39)$$

5.10 MAIN COMPONENTS OF A LASER SYSTEM

A laser requires three main components for operation as shown in Fig. (1.16)

(i) The pumping source or energy source (ii) The active medium (iii) The optical resonator.

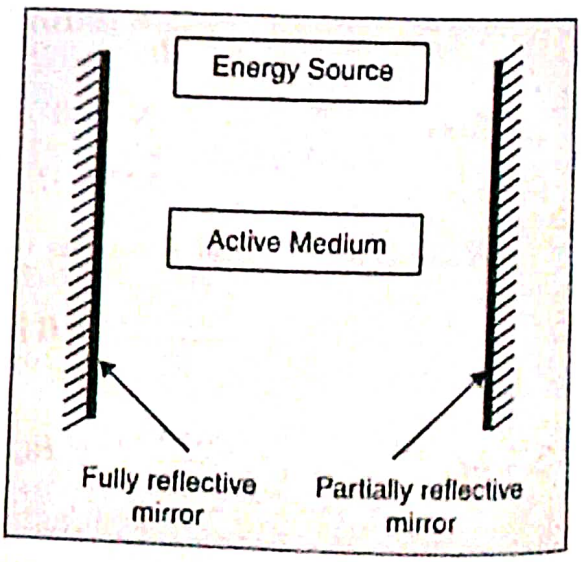


Fig. 1.16

(i) Pumping Source or Energy Source

The pumping source is an external source that supplies energy to the system and helps in obtaining the population inversion. The excitation of the atoms may occur directly or through atom-atom collisions. The pumping source can be optical, electrical or thermal.

(ii) Active Medium

It is the material in which the laser action is made to take place. It may be solid, liquid or gas. Many lasers are named after the material used. For example Ruby laser, He–Ne laser, CO_2 laser. The wavelength of the laser light depends upon the material used. For example the light wavelength of Ruby laser is 694.3 nm, He–Ne laser is 632.8 nm and of CO_2 laser is 10.6 μm. The laser wavelength may extend from ultra-violet region to the infra-red region.

(iii) Optical Resonator

It essentially consists of two mirrors facing each other. The active medium is enclosed by this cavity. One of the mirror is fully reflective i.e. reflection coefficient is very near to (1) and other mirror is partially reflective (i.e. reflection coefficient less than 1) it enables a part of the internally reflecting beam to escape out as laser beam. The resonator is basically a feedback device, that directs the photons back and forth through the laser medium and in the process, the number of photons is multiplied due to stimulated emission.

5.11 RUBY LASER

The first successful laser using ruby crystal was invented by T.H. Maiman in 1940. Ruby belong to family of gems. It is basically Al_2O_3 crystal doped with 0.05% chromium atoms. The active material in the ruby are chromium ions C_r^{+++}. The colour of the ruby crystal depends upon the contents of chromium in it. When ruby crystal contains 0.05% of chromium, its colour is pink. Ruby laser, consists of mainly following parts as shown in Fig. (1.17).

(I) An active Working Material. It is a rod of ruby crystal.

(II) A resonant Cavity. Made of fully reflecting plate at the left of ruby crystal and a partially reflecting plate at the right of ruby crystal. Both the plates are optically plane and exactly parallel to each other.

(III) Pumping Source. A helical xenon flash tube with power supply source.

(IV) Cooling System. Water circulating system in glass tube surrounding it.

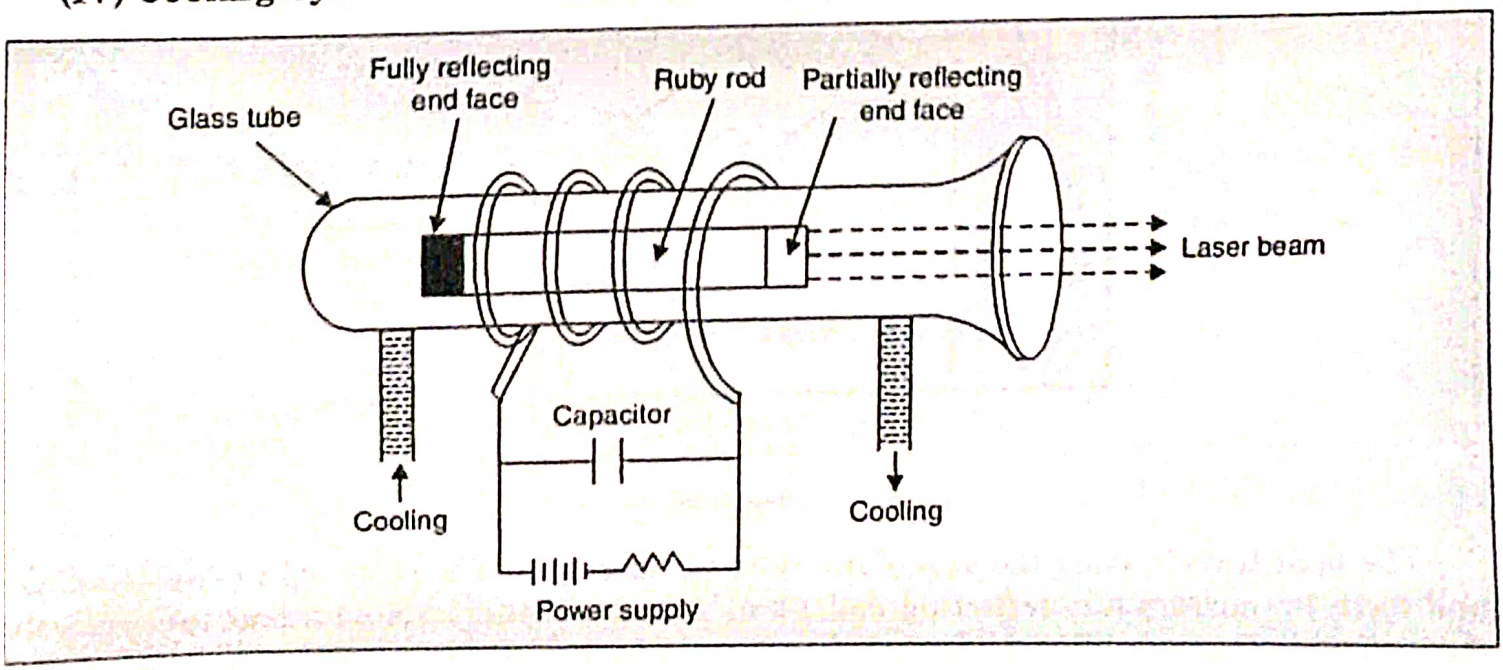


Fig. 1.17

Construction. Ruby crystals are grown in special furnaces with varying length and diameter. In a ruby laser, a pink rod of 4 cm length and 0.5 cm in diameter is generally used. The end faces of the rod are made strictly parallel grounded and polished to high degree. The end faces are then silvered such that one end face becomes fully reflecting while the other end face partially reflecting. The ruby rod is surrounded by a helical xenon flash tube which provides pumping light to raise the chromium ions to upper energy level. Only a part of energy provided by flash lamp is used in pumping the C_r^{+++} ions while the remaining heats up the apparatus. For this purpose a cooling arrangement is used as shown in Fig. (1.17).

Working. Ruby is a three-level laser system. The energy diagram shown in Fig. (1.18) illustrates the operational principle of ruby laser. The energy level of chromium ion C_r^{+++} are shown in Fig. (1.18). There are two main bands called blue bands and green bands. These bands are about 1000Å wide which makes optical pumping effective. The intense light of wavelength 550 nm from flash lamp passes through the ruby. Light excites some of the ruby's atoms. A large fraction of chromium ions in the ground state are excited to an energy level in the blue band (E_1) and green band (E_2). The excited chromium ions quickly lose some of their energy and make radiation less transitions form excited state to the pairs of levels associated with metastable state with 10^{-8} second. This energy is used only by vibrations of atoms in crystal lattice and get dissipated in the from of heat. In metalstable state the chromium ions stay for a long time of the order of milliseconds (10^{-3} sec.). Thus the number of chromium ions in the metastable state becomes ultimately greater than the number in ground state producing population inversion between them. The chromium ions in the metastable state make stimulated emission transitions to the ground state by emitting a sharp doublet of wavelengths 6943 Å and 6928 Å. However laser action takes place only at 6943 Å. The metastable state plays the part of upper laser level. Thus ruby laser is three level laser scheme.

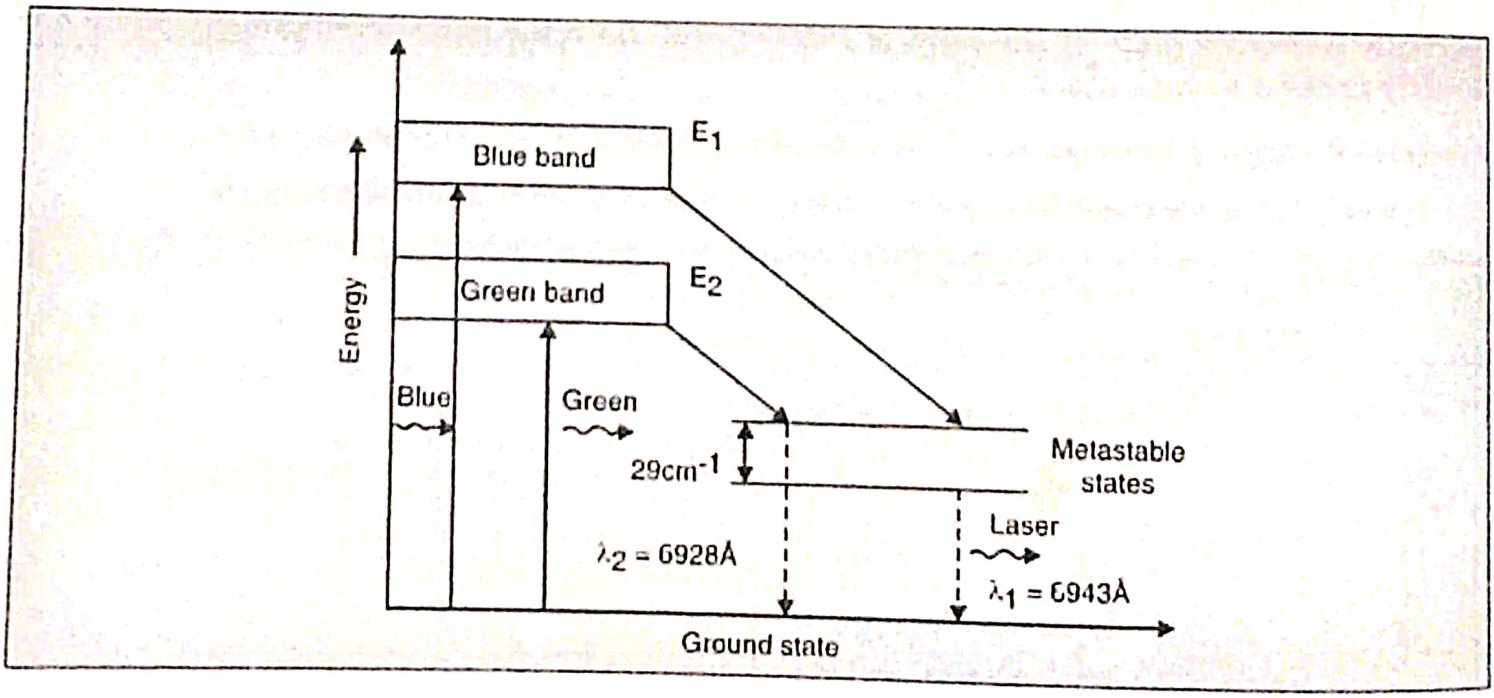


Fig. 1.18

The light travels along the axis of the ruby as laser light. The laser light is reflected back and forth by mirrors (i.e. reflecting ends) and stimulate other excited atoms into releasing their energy. This amplifies the laser light of wavelength 6943 Å.

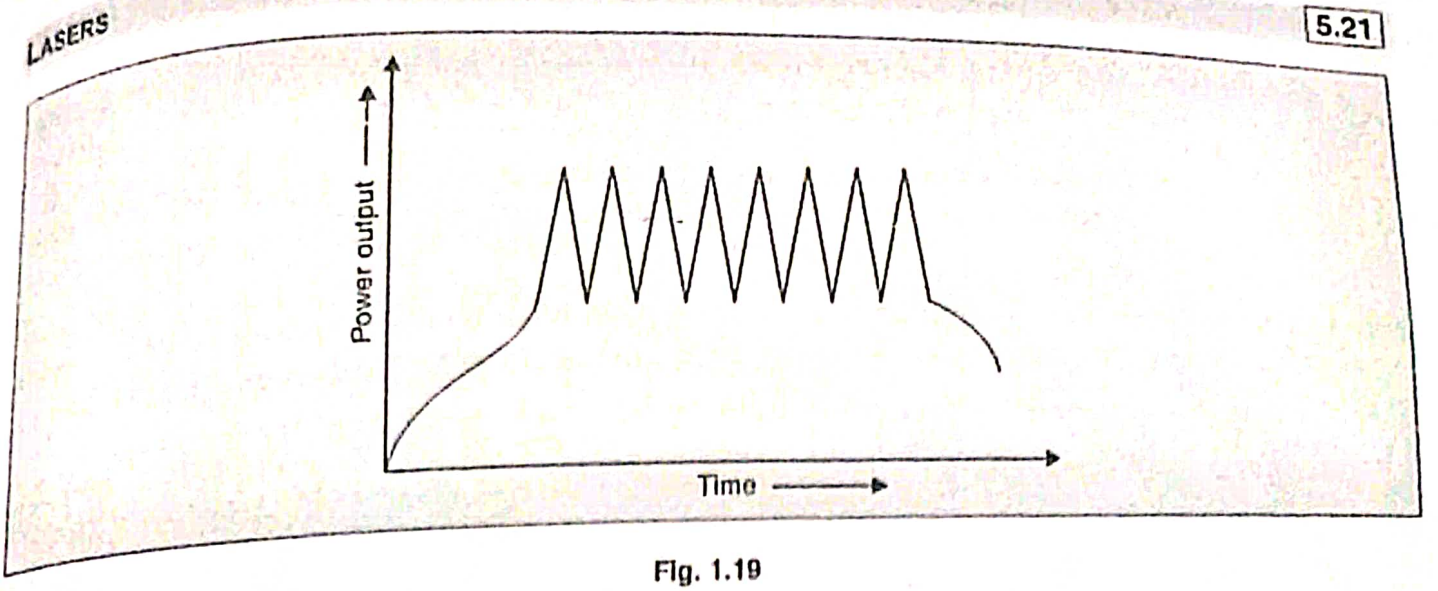


Fig. 1.19

The flash operation of the pump leads to pulsed output of laser. As soon as the flash lamp stops operating, the condition of population inversion is broken. Consequently the lasing action stops till the arrival of the next flash from the lamp. Even in the short period of a few tens of microseconds in which the ruby is lasing, one finds that the emission consists of spikes of high intensity emissions as shown in Fig. (1.19). This phenomena is called spiking.

Drawbacks :

(i) Ruby laser has low laser efficiency.

(ii) The laser requires high pumping power.

(iii) The laser output is not continuous but occurs in the form of pulses of microsecond duration.

(iv) The defects due to crystalline imperfection is also present in this laser.

Advantages/Applications

(i) Ruby laser has very high output power of the order of 10 kW to 1000 kW.

(ii) Ruby lasers are used for holography, industrial cutting and welding.

5.12 HELIUM-NEON LASER

Helium Neon laser was built by AliJavan, *W.* Bennett and *D.* Herriot in 1961. The main characteristics of He-Ne laser are as follows :

(i) It is a four level laser, hence population inversion can be easily obtained.

(ii) The power output of He-Ne laser lies in range 1–50 *MW* with input power 5 Watt to 10 Watt.

(iii) It is capable of supplying continuous laser beam without the need of elaborate cooling arrangement.

(iv) The light from He-Ne is more directional and more monochromatic as compared to that from solid state lasers.

(v) Due to high coherence length and high monochromaticity, the He-Ne is used for alignment, interferrometry, data-processing holography etc.

(vi) The He-Ne laser employs electrical pumping in which there is less wastage of energy as compared to optical pumping methods used in solid state lasers.

Construction. The helum-neon laser consists of a long discharge tube of length 50 cm and diameter 1 cm. The tube contains a mixture of about 10 parts of helium and 1 part of neon at a pressure of about 1 mm of Hg. The gas mixture of helium and neon forms the lasing medium and is enclosed between a set of mirrors forming resonant cavity.

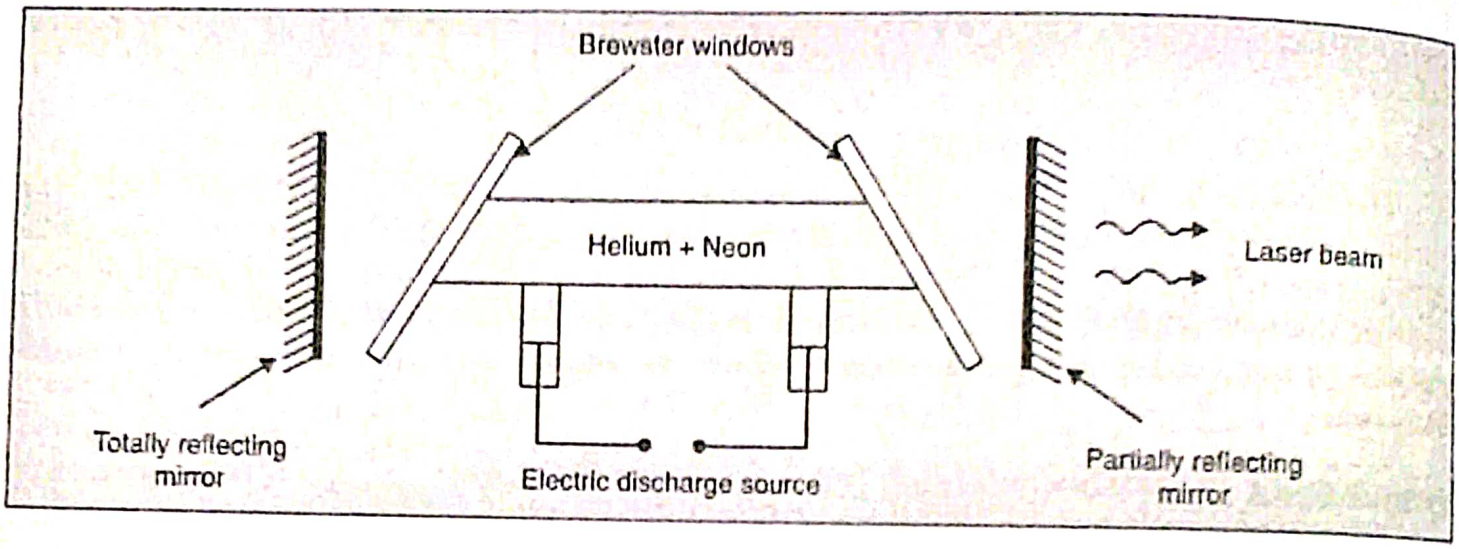


Fig. 1.20

One of the mirrors is completely reflecting and other is partially reflecting, so that laser beam may come out. A stationary glow discharge is excited in the gas by applying few kilovolt d.c. The disadvantage of using mirrors inside the discharge tube is that mirros are eroded with time due to gas discharge and have to be replaced. Also when external mirrors are used then there is loss of light at the ends of the discharge tube due to reflection. To reduce this loss, end faces of the tube are inclined at Brewster's angle. Thus while passing through these windows light, which is polarized in the plane of windows does not suffer reflection while other light suffers reflection. Hence output light beam is plane polarized as shown in Fig. (1.20).

Working : When electric discharge takes place in the gas mixture, some of the atoms of the mixture get ionized. The electrons get accelerated in the discharged tube. These accelerated electrons collide with helium atoms and excite them from level F_1 to levels F_2 and F_3 as shown in Fig. (1.21). The levels F_2 and F_3 happen to be metastable states, thus helium atoms excited to these levels spend a sufficient long time before getting de-excited. Some of the excited states of neon correspond almost to the same energy as the energy of the excited states F_2 and F_3 of helium. Therefore, when helium atoms in levels F_2 and F_3 collide with neon atoms in the ground level E_1, an energy exchange takes place; consequently neon atoms get excited to the levels E_4 and E_6 and helium atoms get de-excited to ground state F_1. Since helium atoms have longer life time in excited states F_2 and F_3 thus this process of energy transfer has high probability. Therefore, the electric discharge through the gas mixture continuously populates the neon excited levels E_4 and E_6. This creates a state of population inversion between levels E_4 (or E_6) and lower energy levels E_5 and E_3. Following transitions occurs as shown in fig. (5.21).

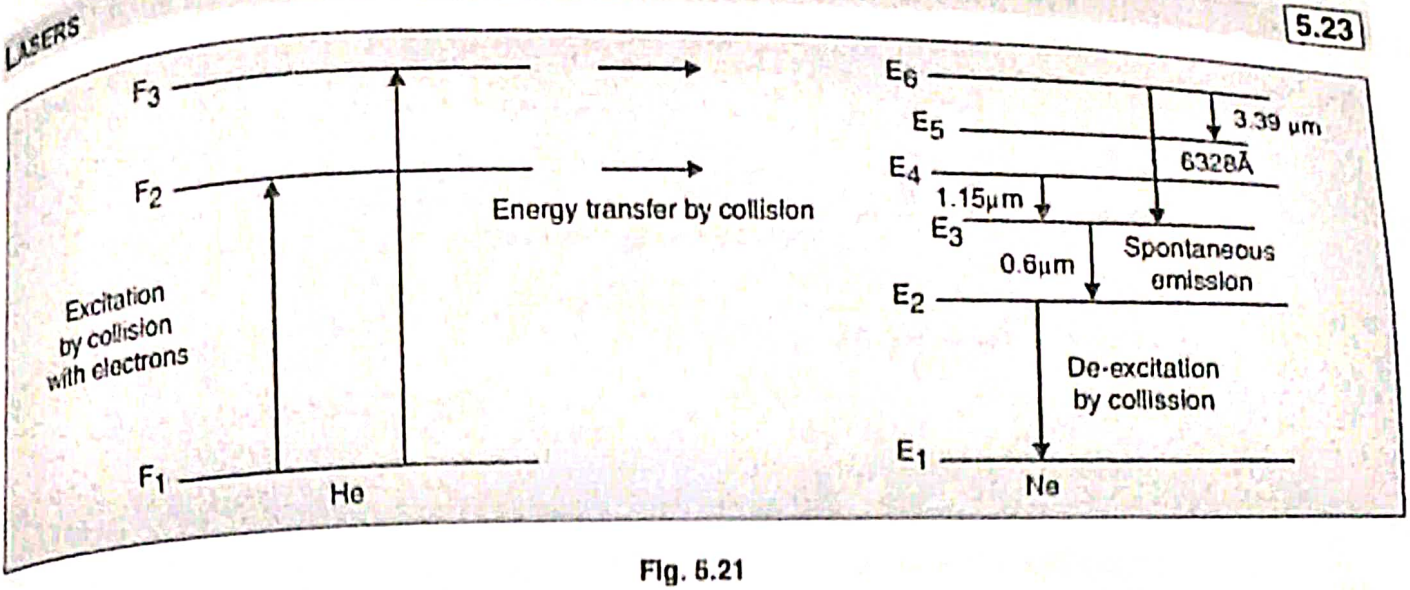


Fig. 6.21

From level E_6 to E_5 with laser wavelength 3.39 μm, from level E_6 to E_3 with laser wavelength 6328Å and from level E_4 to E_3 with laser wavelength 1.15 μm. The wavelengths 3.39 μm and 1.15 μm correspond to infrared region where as 6328Å corresponds to red light. Mirrors of the optical resonators are so designed to have low reflectivity for wavelengths 3.39 μm and 1.15 μm. Thus photons of these wave lengths will be eliminated. Therefore, the photons of wavelength 6328Å will move back and forth in optical resonator system and thus laser of wavelength 6328 Å emerges through the partially reflecting mirror.

The excited neon atoms de-excite from level E_3 to E_2 by spontaneous emission and emits a photon of wavelength 0.6 μm. As the level E_2 is also a metastable state, there is a probability of excitation of neon atoms from E_2 to E_3 leading to the quenching the population inversion. To eliminate quenching, the narrow discharge tube is used because Ne atoms de-excited to level E_1 from E_2 through collisions with the walls of the tube.

The output of He-Ne laser is continuous and lies between/1mW and 50 mW for input of about 5 to 10 W.

Applications. He-Ne lasers are used in research, spectroscopy, holography, communications and weaponry.

SOLVED PROBLEMS

PROBLEM 1. Calculate the temporal coherence length for Ruby laser operating at wavelength 6943Å. Given emission band width = 10^6 Hz.

Solution

Here $\lambda = 6943\text{Å} = 6943 \times 10^{-10}$ m

$\Delta\nu = 10^6$ Hz

Coherence $L = cT$ $= CT$

Also $\Delta\omega = \dfrac{2\pi}{T}$ or $2\pi\Delta\nu = \dfrac{2\pi}{T}$

or $\Delta\nu = \dfrac{1}{T}$ or $T = \dfrac{1}{\Delta\nu}$

$$\therefore \quad L = \frac{c}{\Delta\nu} \qquad \ldots(1)$$

Since $\nu = \frac{c}{\lambda}$ or $\Delta\nu = -\frac{c}{\lambda^2}\Delta\lambda$

or $\Delta\nu = \frac{c}{\lambda^2}\Delta\lambda$ (Neglecting –ve sign)

$$\therefore \quad L = \frac{c\lambda^2}{c\Delta\lambda} = \frac{\lambda^2}{\Delta\lambda} \qquad \ldots(2)$$

From eqs. (1) and (2)

$$\frac{c}{\Delta\nu} = \frac{\lambda^2}{\Delta\lambda}$$

or $$\Delta\lambda = \frac{\lambda^2}{c}\Delta\nu$$

$$= \frac{(6943\times10^{-10})^2}{3\times10^8}\times10^6$$

$$= \frac{6943\times6943\times10^{-14}}{3\times10^8} = 1.6\times10^{-15}\,m$$

$\therefore$ Coherence length $= L = \frac{\lambda^2}{\Delta\lambda}$

$$= \frac{(6943\times10^{-10})^2}{1.6\times10^{-15}} = 301\ m$$

PROBLEM 2. **Find the coherence length for white light, the wavelength of white light ranges from 4000Å to 7000 Å ?**

Solution

Here $\Delta\lambda = (7000 - 4000)\text{Å} = 3000\text{Å} = 3000 \times 10^{-10}\ m = 3 \times 10^{-7}\ m$

Average wavelength $\lambda = \frac{7000+4000}{2} = 5500\text{Å}$

$$= 5500 \times 10^{-10}\ \text{m} = 55 \times 10^{-8}\ m$$

Coherence length $= L = \frac{\lambda^2}{\Delta\lambda} = \frac{(55\times10^{-8})^2}{3\times10^{-7}} = \frac{55\times55\times10^{-16}}{3\times10^{-7}}$

$$= \frac{3025}{3}\times10^{-9} = 1008.3 \times 10^{-9}\ m$$

$$= 10083 \times 10^{-10}\ m = 10083\ \text{Å}$$

PROBLEM 3. **The sodium yellow light of wavelength $\lambda = 5893$Å is doublet of 6 Å width. Calculate its coherence length and coherence time. Also find its non-monochromaticity.**

Solution

Here $\lambda = 5983$ Å $= 5893 \times 10^{-10}$ *m*

$\Delta\lambda = 6$Å $= 6 \times 10^{-10}$ *m*

Coherence length $L = \dfrac{\lambda^2}{\Delta\lambda}$

$$= \frac{(5893\times10^{-10})^2}{6\times10^{-10}} = \frac{(5983)^2}{6}\times10^{-10}$$

$$= \frac{34727449}{6}\times10^{-10} = 5787908.2 \times 10^{-10}\ m$$

$$= 5.79 \times 10^{-4}\ m$$

Coherence time $T_c = \dfrac{L}{c} = \dfrac{5.79\times10^{-4}}{3\times10^{8}} = 1.93 \times 10^{-12}$ sec.

Non-monochromaticity

$$\frac{\Delta\nu}{\nu} = \frac{\Delta\lambda}{\lambda}$$

$$= \frac{6\times10^{-10}}{5893\times10^{-10}} = 1.01 \times 10^{-3}$$

PROBLEM 4. **A source of light of wavelength, $\lambda = 6 \times 10^{-5}$ cm subtends an angle of 30′. Find its lateral coherence width.**

Solution

Here $\lambda = 6 \times 10^{-5}$ *cm*, $\theta = 30' = \dfrac{\pi\times30}{180\times60}$ radians.

$$= \frac{22\times30}{7\times180\times60} = \frac{22}{7\times180\times2}$$

$$= \frac{11}{7\times180} = \frac{11}{1260} = 0.0087 \text{ rad.}$$

Lateral coherence width

$$= \frac{\lambda}{\theta} = \frac{6\times10^{-5}}{0.0087} = 689.65\times10^{-5}$$

$$\approx 6.89 \times 10^{-3} \text{ cm}$$

PROBLEM 5. For an ordinary source the coherence time $T_c \approx 10^{-10}$ sec. Calculate the degree of non-monochromaticity $\left(\frac{\Delta\nu}{\nu}\right)$ for wavelength 5500Å.

Solution

Here $T_c = 10^{-10}$ sec $\lambda = 5500\ A^\circ = 5500 \times 10^{-10}\ m$

$= 55 \times 10^{-8}\ m$

$$\Delta\nu = \frac{1}{T_c} = \frac{1}{10^{-10}} = 10^{10}\ Hz$$

$$\nu = \frac{c}{\lambda} = \frac{3\times10^8}{55\times10^{-8}} = 0.0545 \times 10^{16} = 545 \times 10^{12}\ Hz$$

Degree of non-monochromaticity $= \left(\frac{\Delta\nu}{\nu}\right)$

$$= \frac{10^{10}}{545\times10^{12}} = 0.00183 \times 10^{-2}$$

$$= 183 \times 10^{-7}$$

PROBLEM 6. Find the coherence length of a laser source of monochromatic light with frequency width of 1200 *Hz*.

Solution

Here $\Delta\nu = 1200\ Hz$

Coherence Time $T_c = \frac{1}{\Delta\nu} = \frac{1}{1200} = \frac{1}{12}\times10^{-2}$ sec.

Coherence Length $L = cT_c = 3 \times 10^8 \times \frac{1}{12}\times10^{-2} = \frac{1}{4}\times10^6$

$= 0.25 \times 10^6\ m = 250 \times 10^3\ m = 250\ km$

PROBLEM 7. What is the transition rate for the neon atom in a He-Ne laser, if the energy drop for the 6328Å emission is 1.96 *eV* and the power output is 10^{-3} watts.

Solution

Here Power output $(P) = 10^{-3}$ watt, $\lambda = 6328$ Å $= 6328 \times 10^{-10}\ m$

Transition rate for neon atom $= \frac{\text{Power}}{\text{Energy}}$

$$= \frac{P}{h\nu} = \frac{P\lambda}{hc}$$

$$= \frac{10^{-3} \times 6328 \times 10^{-10}}{6.63 \times 10^{-34} \times 3 \times 10^{8}}$$

$$= 3.18 \times 10^{13}/\text{sec.}$$

PROBLEM 8. **Find the intensity of a laser beam of 10 mW power and having a diameter of 1.2 $m.m$. Assume the intensity to be uniform across the beam.**

Solution

Here $P = 10\ mW = 10 \times 10^{-3}$ watt $= 10^{-2}$ watt

$D = 1.2\ mm = 1.2 \times 10^{-3}\ m$

$$\text{Intensity} = \frac{\text{Power}}{\text{Area}} = \frac{4P}{\pi d^2} = \frac{4 \times 10^{-2}}{3.14 \times (1.2 \times 10^{-3})^2} = \frac{4 \times 10^{-2}}{3.14 \times 1.44 \times 10^{-6}}$$

$$= \frac{4}{4.52} \times 10^{4} = 0.8849 \times 10^{4} = 8849\ \frac{W}{m^2} = 8.85 \frac{kW}{m^2}$$

PROBLEM 9. **A certain ruby laser emits 1.0 J pulses of light per sec. whose wavelength is 6940Å. What is the minimum number of C_r^{+++} ions in the ruby ?**

Solution

Here $P = 1.0$ J/s, $\lambda = 6940$ Å $= 6940 \times 10^{-10}\ m$

$$P = \frac{nhc}{\lambda t} = \frac{nhc}{\lambda}$$ (i.e. Power = No. of ions × Energy of one photon)

(Here $t = 1$ sec.)

or $$n = \frac{P\lambda}{hc}$$

$$= \frac{1 \times 6940 \times 10^{-10}}{6.62 \times 10^{-34} \times 3 \times 10^{8}}$$

$$= \frac{6940}{19.86} \times 10^{16} = 349 \times 10^{16}$$

$$= 3.49 \times 10^{18} \text{ ions}$$

PROBLEM 10. **A laser beam can be focussed on an area equal to the square of its wavelength (λ^2). For a He-Ne laser $\lambda = 6328$ A°. If the laser radiates energy at a rate of 1 mW, find out the intensity of focused beam.**

Solution

Here $\lambda = 6328\ A° = 6328 \times 10^{-10}\ m$

$P = 1\ mW = 10^{-3}\ W$

$$A = \lambda^2 = (6328 \times 10^{-10})^2 = 40 \times 10^{-14}\ m^2$$

$$\text{Intensity} = \frac{P}{A} = \frac{10^{-3}}{40 \times 10^{-14}} = 2.5 \times 10^{9}\ W/m^2$$

PROBLEM 11. Calculate the energy and momentum of a photon of a laser beam of wavelength 6328 Å.

Solution

Here $\lambda = 6328\ Å = 6328 \times 10^{-10}\ m$

$$\text{Energy of a photon } E = h\nu = \frac{hc}{\lambda} = \frac{(6.62 \times 10^{-34}) \times (3 \times 10^{8})}{6328 \times 10^{-10}}$$

$$= 3.14 \times 10^{-19}\ J = \frac{3.14 \times 10^{-19}}{1.6 \times 10^{-19}}\ eV = 1.96\ eV$$

$$\text{Momentum of photon } p = \frac{h}{\lambda} = \frac{6.62 \times 10^{-34}}{6328 \times 10^{-10}} = 1.05 \times 10^{-27}\ kgm/s$$

CONCEPTUAL QUESTIONS

Q. 1. Why population inversion is essential for stimulated emission ?

Ans. Because the rate of stimulated emission can be more than stimulated absorption, only by achieving population inversion.

Q. 2. What do you mean by the life time of an energy state ?

Ans. Life time of an energy state is defined as the time in which number of atoms in that state becomes $\frac{1}{e}$ times the initial number of atoms in that state. It is measure of time for which an atom remains in that state.

Q. 3. Define (i) Coherence time and (ii) Coherence length.

Ans. (i) **Coherence time** (T_c). The average time interval during which the phase difference of the wave remains constant, is called the coherence time.

(ii) Coherence length. If c is the speed of light, then the length covered by the wave in coherence time is known as coherence length.

Coherence length = Coherence time × c

$$L = T_c \times c$$

Q. 4. Explain the term pumping.

Ans. Population inversion in obtained by pumping. Raising the atoms to the higher energy state is called pumping. This can be done by optical pumping in ruby laser or by using an electric discharge in He-Ne laser. In three level laser atoms will be pumped to

excited level E_3 from level E_1 and in four level laser the atoms will be pumped to excited level E_4 from level E_1.

Q. 5. Can we obtain light amplification in the absence of stimulated emission?

Ans. No, only in the case of stimulated emission, we obtain photons of the same phase, energy, frequency, state of polarization and travel to each other. They constitute the coherence radiation which superimpose to produce radiations of very high intensity.

Q. 6. Define quantum efficiency. Can a laser have 100% efficiency ?

Ans. Quantum efficiency of a laser is defined as

$$\eta = \frac{\text{Ouput Energy}}{\text{Input Energy}}$$

For a two level laser quantum efficiency is given as

$$\eta = \frac{E_2 - E_1}{E_2 - E_1} = 1$$

Hence two level laser has 100% efficiency.

Q. 7. Which of the laser is more efficient : two level, three level or four level ? Explain.

Ans. Quantum efficiency of two level laser is given as

$$\eta = \frac{E_2 - E_1}{E_2 - E_1} = 1$$

i.e. η is 100% for level laser

Quantum efficiency of three level laser is given as

$$\eta = \frac{E_2 - E_1}{E_3 - E_1} < 1$$

i.e. $\eta < 100\%$ for three level laser

Quantum efficiency of four level laser is given as

$$\eta = \frac{E_3 - E_2}{E_4 - E_1} < 1$$

i.e. $\eta < 100\%$ for four level laser

Hence quantum efficiency of two level laser > three level laser > four level laser.

$\therefore$ Two level laser is most efficient.

Q. 8. Why optical pumping cannot be used for gas lasers ?

Ans. It is because of the fact that there are no energy bands in gases. Since optical flash lamp gives highly intense pulses of polychromatic light, so only those radiations will be absorbed by gas molecules, whose energy is exactly equal to the difference in energies of ground and excited state. Hence optical pumping cannot be used for gas lasers.

Q. 9. What do you understand by metastable state ?

Ans. Normally, the mean life of excited atoms before spontaneous emission is 10^{-8} second. However, for some excited states, this mean life is about 10^{5} times. We call such long lived states metastable. They occupy an important role in laser action.

Q. 10. What is the wavelength of laser light from (i) Ruby laser and (ii) He-Ne laser ? How are two lasers different ?

Ans. (i) Wavelength of Ruby laser is 6943Å and

(ii) Wavelength of He-Ne laser is 6328Å.

Ruby laser is a three level laser and has pulsed output, where as he-Ne laser is a four level laser and has continuous output.

Q. 11. Which laser is better either Ruby or He-Ne laser ? Why ?

Ans. He-Ne laser. The output of Ruby laser is in the form of pulses. He-Ne laser is better than Ruby laser because

(i) it has continuous output (ii) being a four level laser, laser action is fast in it (iii) its active material is relatively cheaper.

Q. 12. What is an active medium ?

Ans. A medium in which population inversion is achieved for laser action is called an active medium.

Q. 13. What is an optical resonator ?

Ans. It is a pair of reflecting surfaces (mirrors) of which one is perfect reflector and other is partial reflector. It is used for amplification of photons and hence producing an intense and highly coherent output.

Q. 14. State whether a laser is an amplifier or an oscillator ?

Ans. The mirrors in a resonator provide positive feedback to the photons amplified in the active medium. In analogy with electric oscillator (in which a part of output voltage is feedback to the input in proper phase i.e. positive feedback), the laser is an amplifier.

Q. 15. In He-Ne laser, lasing is through neon gas. What is then the role of helium ?

Ans. In He-Ne laser, helium serves as a buffer gas and helps in the excitation of neon atoms. Since He atoms are much lighter than Ne-atoms, electrons transfer energy more readily to He atoms. The excited He-atoms in turn transfer this energy to Ne-atoms.

Q. 16. Why cooling is required in Ruby laser ?

Ans. In Ruby laser we use xenon flash tube in which each flash lasts several milliseconds and in each flash a few thousand joules of energy is consumed. Since the xenon discharge gives white light radiations and Ruby laser is a three level system, only a part of energy for pumping process i.e. in exciting the Cr^{+++} ions. The rest of energy heat up the apparatus and hence the cooling is required in Ruby laser.

Q. 17. Why is it necessary to use a narrow tube in a He-Ne laser ?

Ans. A narrow discharge tube is necessary for rapid de-excitation of atom by collision with the walls. With a tube of large diameter, the probability of collisions of atoms with the walls decreases and less atoms are available at the ground level for further excitation. This can cease the laser action in due course.

MULTIPLE CHOICE QUESTIONS

1. **LASER is abbreviation used for :**
   (a) name of scientist
   (b) light amplification by stimulated emission of radiation
   (c) light amplification by spontaneous emission of radiation
   (d) light absorption by sun and earth radiation.

2. **A laser is coherent source because it contains :**
   (a) many wavelengths
   (b) uncoordinated wave of a particular wavelength
   (c) coordinated wave of a particular wavelength
   (d) none of these.

3. **The ratio of probabilities of spontaneous emission and stimulated emission is directly proportional to :**
   (a) frequency ν (b) ν^2
   (c) ν^3 (d) ν^4

4. **The directionality of a laser beam is measured by :**
   (a) visibility of interference fringes
   (b) the size and aperture of laser source
   (c) the divergence angle of the beam with the distance from source
   (d) nature of the lasing medium

5. **Laser beam is monochromatic. It means, it has :**
   (a) single frequency (b) narrow width
   (c) wide width (d) several colours

6. **Population inversion in helium neon laser is produced by :**
   (a) photon excitation (b) chemical excitation
   (c) inelastic atomic collisions (d) chemical reaction

7. **In He-Ne laser, the most favourable ratio of helium to neon for satisfactory laser action is :**
   (a) 1 : 7 (b) 7 : 1
   (c) 1 : 10 (d) 10 : 1

8. **Helium-Neon laser emits light of :**

(a) wavelength of 3.39 μm only (b) wavelength of 1.15 μm only

(c) wavelength 6328 Å only (d) all of them

9. **Which of the following is active medium for Rub laser :**

(a) Cr_2O_3 (b) Al_2O_3

(c) Chromium atoms (d) Chromium ions

10. **The lasers are classified :**

(a) according to size and shape of resonator

(b) according to the state of laser medium and according to the nature of output

(c) according to type of pumping

(d) all of them.

11. **Which of the following is the three level Laser system :**

(a) He-Ne laser (b) *Nd* : YAG laser

(c) Semiconductor laser (d) Ruby laser

12. **The ratio of Einstein's coefficients *A* and *B* can be expressed as :**

(a) $\frac{8\pi hc^3}{\nu^3}$ (b) $\frac{8\pi hc}{\nu^3}$

(c) $\frac{8\pi hc^3}{\nu}$ (d) $\frac{8\pi h\nu^3}{c^3}$

13. **Laser beam is highly coherent, so it can be used in :**

(a) interference (b) diffraction

(c) polarisation (d) following

14. **Which is not true for LASER, in the following :**

(a) extremely intense light (b) perfectly monochromatic

(c) coherent (d) divergent

15. **A laser light consists of :**

(a) electron beam

(b) proton beam

(c) perfectly coherent photon

(d) perfectly coherent phonons

Answers

1.	(b)	2.	(c)	3.	(c)	4.	(c)	5.	(a)
6.	(c)	7.	(d)	8.	(d)	9.	(c)	10	(b)
11.	(d)	12.	(d)	13.	(a)	14.	(d)	15.	(c)

CHAPTER AT A GLANCE

1. LASER is the abbreviation stands for "Light Amplification by Stimulated Emission of Radiation.".

2. Characteristics of laser light

(i) Directionality (ii) High intensity (iii) High degree of coherence and (iv) Extraordinary monochromaticity.

3. Stimulated absorption

When an atom in the ground state with energy E_1 absorbs a photon of incident radiation, it gets excited to the higher energy state E_2. Then energy absorbed is given as

$$h\nu = E_2 - E_1$$

This process is called stimulated absorption or simply absorption.

4. Spontaneous emission

When an atom in the excited state E_2 gets de-excited to the ground state E_1 by emitting a photon of energy $h\nu$

$$h\nu = E_2 - E_1$$

This type of emission is called spontaneous emission.

5. Stimulated emission

Stimulated emission is the process in which an incident photon of appropriate frequency triggers an atom in the excited state to emit radiation.

6. Following are Einstein's coefficient

B_{12} = Einstein's coefficient for absorption of radiation

A_{21} = Einstein's coefficient of spontaneous emission of radiation.

B_{21} = Einstein's coefficient for stimulated emission of radiation.

Further $B_{21} = B_{12}$ and

$$\frac{A_{21}}{B_{21}} = \left(\frac{8\pi h\nu^3}{c^3}\right)\alpha\,\nu^3$$

7. Population inversion and metastable states

The process of achieving greater population density. (*i.e.*number of atoms per unit volume) in the higher energy state as compared to lower energy state is called population inversion. The population inversion is possible only in those substances which have meta-stable states.

8. Pumping. The process of achieving population inversion by supplying external energy by any means is called pumping.

Following methods may be used for pumping :

(i) Optical pumping (ii) Electric discharge (iii) Direct conversion (iv) Chemical reactions (v) Inelastic atom-atom collisions.

9. Various level laser systems

(i) Two level laser system. In this case only two levels are involved in laser action. Quantum efficiency for two level laser system is given as

$$\eta = \frac{E_2 - E_1}{E_2 - E_2} = 1$$

(ii) Three level laser system. In this case three energy levels are involved in laser action. Quantum efficiency for three level laser system is given as

$$\eta = \frac{E_2 - E_1}{E_3 - E_1} < 1$$

(iii) Four level laser system. In this case four energy levels are involved in laser action. Quantum efficiency for four level laser system is given as

$$\eta = \frac{E_3 - E_2}{E_4 - E_1} < 1$$

10. Main Components of a laser system are :

(i) Active medium (ii) Pumping source and (iii) Optical resonator.

11. Ruby laser. The working substance in Ruby laser is a crystal Al_2O_3. The optical pumping is used. The ruby laser is a pulsed laser beam.

12. Helium-Neon laser. The working substance is a mixture of helium and neon gases. The optical pumping system is gaseous discharge. This excites helium atoms which in turn collide with unexcited neon-atoms and force them to excited state. In this way population inversion is achieved. It emits a continuous laser beam.

13. Laser beams are used in communication, computers, industry, medicine, military and holography etc.

SHORT ANSWER QUESTIONS

1. What do you mean by the term 'LASER' ?
2. What is basic principle of LASER ?
3. What is population inversion and why it is important for lasing ?
4. Why it is easy to use two-level atom in laser ?
5. Are there any two level atom laser ? What are they ?
6. What do you mean by stimulated absorption of light ?
7. What is stimulated emission of light ?
8. What is the need of stimulated emission of light ?
9. What do you mean by the term population inversion ?
10. What do you mean by pumping ?
11. What do you mean by optical pumping ?
12. What is difference between the continuous and pulsed laser output ?

13. Who made the first Ruby laser ? What is its output wavelength ?
14. Why is the ruby laser not very efficient ?
15. Who made He-Ne laser ? What is its output wavelength ?
16. Give an example of a three level laser.
17. Give an example of a four level laser.
18. Why laser light is more directional than the ordinary light ?
19. Why focusing of laser light is better than ordinary light ?
20. Can we obtain light amplification in the absence of stimulated emission ?

LONG ANSWER QUESTIONS

1. What are the properties of laser light ?
2. Write four properties of laser light.
3. What do you mean by spatial coherence and temporal coherence ? Explain.
4. Explain the mechanism of production of laser beam.
5. Explain the following terms :

   (i) Spontaneous emission (ii) Stimulated emission (iii) Population inversion (iv) Metastable state
6. What are the characteristics that distinguish laser from ordinary source of light?
7. Explain directionality and monochromaticity for laser light.
8. Distinguish between spontaneous and stimulated emissions. Which one of the two predominates in optical region at room temperature ?
9. Discuss in details the concept of directionality, monochromaticity, intensity and coherence of laser light.
10. What do you understand by spatial and temporal coherence of light source ? What is coherence time and coherence length ?
11. Define coherence, temporal coherence, spatial coherence, coherence time and coherence length.
12. What are Einstein coefficients ? Show that they are related as

$$B_{12} = B_{21} \text{ and } \frac{A_{21}}{B_{21}} = \frac{8\pi h\nu^3}{c^3}$$

13. Explain the terms (i) Life time of an energy level (ii) Metastable states (iii) Optical pumping and (iv) Population inversion.
14. Explain (i) Three level laser and (ii) Four level laser schemes.
15. Explain why we prefer four level laser over three level laser even if its efficiency is low ?
16. Explain working principle and construction of Ruby laser.

17. Draw a neat diagram to represent the components of a Ruby laser. Explain its operation.
18. Explain the working, construction and energy level diagram for Ruby laser. Explain spiking in Ruby laser.
19. What are Einstein's coefficients ? Derive a relation between Einstein's spontaneous and stimulated emission coefficients.
20. Explain Einstein's coefficients and derive an expression for finding the ratio of these coefficients.
21. Explain the principle, construction and working of a He-Ne laser.
22. Discuss with suitable diagrams, the principle, construction and working of He-Ne laser. Give its two applications.
23. What is the role played by He in a He-Ne laser ? Explain using an energy level diagram.

UNSOLVED NUMERICAL PROBLEMS

1. Light of wavelength 4800Å has a length of 25 waves, what is coherence length and coherence time ? [**Ans.** $12 \times 10^{-6}\ m$, $4 \times 10^{-14}\ s$]

   [**Hints.** $\lambda = 4800Å = 4800 \times 10^{-10}\ m$, $L = 25 \times 4{,}800 \times 10^{-10}\ m = 12 \times 10^{-6}\ m$, $T_c = \frac{L}{c} = \frac{12\times10^{-6}}{3\times10^{8}} = 4\times10^{-14}\ s$]

2. Calculate the coherence length for CO_2 laser whose width is $10^{-5}\ mm$ at *IR* emission wavelength of 10.6 μm. [**Ans.** 11.2 *km*]

   [**Hints.** $\lambda = 10.6\ \mu m = 10.6 \times 10^{-6}\ m$, $\Delta\lambda = 10^{-5}\ mm = 10^{-5} \times 10^{-3}\ m = 10^{-8}\ m$, $L = \frac{\lambda^2}{\Delta\lambda} = \frac{(10.6\times10^{-6})^2}{10^{-8}} = 11.2\ km$]

3. The coherence length for sodium D_2 line is 2.5 *cm*. Deduce (i) the coherence time (T_c) and (ii) the spectral width of the line. Given wavelength of D_2 line of sodium is 5896Å. [**Ans.** 8×10^{-11} sec, 1.39×10^{-9} cm]

   [**Hints.** $\lambda = 5896\ Å = 5896 \times 10^{-8}$ cm, $T_c = \frac{L}{c} = \frac{2.5}{3\times10^{10}} = 8\times10^{-11}$ sec, $L = 2.5$ cm, $\Delta\lambda = \frac{\lambda^2}{L} = \frac{(5896\times10^{-8})^2}{2.5} = 1.39\times10^{-9}\ cm$]

4. Calculate the coherence time and coherence length of white light of wavelength range from 3500Å to 6500Å. [**Ans.** 2.52×10^{-15} sec, 7.56×10^{-7} m]

   [**Hints.** $\nu_1 = \frac{c}{\lambda_1} = \frac{3\times10^{8}}{3500\times10^{-10}} = 8.57\times10^{14}\ Hz$, $\nu_2 = \frac{c}{\lambda_2} = \frac{3\times10^{8}}{6500\times10^{-10}} = 4.61\times10^{14}\ Hz$,

$\Delta\nu = \nu_1 - \nu_2 = (8.57 - 4.61) \times 10^{14} = 3.96 \times 10^{14}$ *Hz*, $T_c = \frac{1}{\Delta\nu} = \frac{1}{3.96 \times 10^{14}} = 2.52 \times 10^{-15}$ sec,

$L = cT_c = 3 \times 10^8 \times 2.52 \times 10^{-15} = 7.56 \times 10^{-7}$ *m*]

5. Find how many photons are required per sec. to produce laser beam of $3mW$, when wavelength of laser light is 6943 Å ? [Ans. 1.048×10^{16}]

[Hints. $P = \frac{nh\nu}{\lambda \times t}$ here time = 1 sec, $P = \frac{nhc}{\lambda}$, $n = \frac{P\lambda}{hc} = \frac{3 \times 10^{-3} \times 6943 \times 10^{-10}}{6.62 \times 10^{-34} \times 3 \times 10^8}$

$= 1.048 \times 10^{16}$]

6. Find the intensity of a laser beam of 20 mW power and having a diameter of 1.3 mm. Assuming intensity to be uniform across the beam. [Ans. 1.5 kW/m^2]

[Hints. $P = 20\ mW = 20 \times 10^{-3}\ W$, $d = 1.3\ mm = 1.3 \times 10^{-3}\ m$, $I = \frac{P}{A} = \frac{4P}{\pi d^2}$

$= \frac{4 \times 20 \times 10^{-3}}{3.14 \times (1.3 \times 10^{-3})^2} = 1.5\ kW/m^2$]

7. A certain ruby laser emits 0.8 J pulses of light. There are 4×10^{18} ions of Cr^{+++} in the ruby. Calculate wavelength of the ruby laser. [Ans. 9930Å]

[Hints. $P = \frac{nhc}{\lambda}$ or $\lambda = \frac{nhc}{P} = \frac{4 \times 10^8 \times 6.62 \times 10^{-34} \times 3 \times 10^8}{0.8} = 9930$Å]

8. Determine the wavelength of radiation given out by a laser with energy of $3eV$, given $h = 6.63 \times 10^{-34}$ *J-s* and $c = 3 \times 10^8$ *m/s*. [Ans. 4.14×10^{-7} *m*]

[Hints. $E = h\nu = 3eV = 3 \times 1.6 \times 10^{-19}\ J = 4.8 \times 10^{-19}\ J$, $E = h\nu = \frac{hc}{\lambda}$

or $\lambda = \frac{hc}{E} = \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{4.8 \times 10^{-19}} = 4.14 \times 10^{-7}\ m$]

9. The energy flux of a laser beam is 12 W/cm^2. It falls on 1.5 cm^2 of the surface of the ideal reflecting mirror for 50 minutes. Calculate the momentum transferred and force exerted on the mirror. [Ans. 12×10^{-4} *kgm/s*, 4×10^{-7} *N*]

[Hints. Energy on mirror (E) = $12 W/cm^2 \times 1.5\ cm^2 = 18\ W$,

Momentum transferred $p = \frac{2E}{c} = \frac{2 \times 18 \times 10^4}{3 \times 10^8} = 12 \times 10^{-4}$ *kg m/s*,

Force = $\frac{p}{t} = \frac{12 \times 10^{-4}}{50 \times 60} = \frac{12 \times 10^{-4}}{3000} = 4 \times 10^{-7}\ N$]

□□□

Syllabus

ALL INDIAN UNIVERSITIES & AUTONOMOUS COLLEGES, ODISHA

Physics- XII: Solid State Physics

(Credits; Theory-04) *Theory : 40 Classes (1 hr duration)*

UNIT – I

Crystal Structure: Solids : Amorphous and Crystalline Materials. Lattice Translation Vectors. Lattice with a Basis – Central and Non-Central Elements. Unit Cell. Miller Indices. Types of Lattices, Reciprocal Lattice. Brillouin Zones. Diffraction of X-rays by Crystals. Bragg's Law. Atomic and Geometrical Factor.

Elementary Lattice Dynamics: Lattice Vibrations and Phonons: Linear Monoatomic and Diatomic Chains. Acoustical and Optical Phonons. Qualitative Description of the Phonon Spectrum in Solids. Dulong and Petit's Law, Einstein and Debye theories of specific heat of solids. T^3 law

UNIT – II

Magnetic Properties of Matter: Dia-, Para-, Ferri- and Ferromagnetic Materials. Classical Langevin Theory of dia-and Paramagnetic Domains. Curie's law, Weiss's Theory of Ferromagnetism and Ferromagnetic Domains. Discussion of B-H Curve. Hysteresis and Energy Loss.

Dielectric Properties of Materials: Polarization. Local Electric Field at an Atom. Depolarization Field. Electric Susceptibility. Polarizability. Clausius Mosotti Equation. Classical Theory of Electric Polarizability.

Lasers: Einstein's A and B coefficients. Metastable states. Spontaneous and Stimulated emissions. Optical Pumping and Population Inversion. Three–Level and Four-Level Lasers. Ruby Laser and He-Ne Laser.

UNIT – III

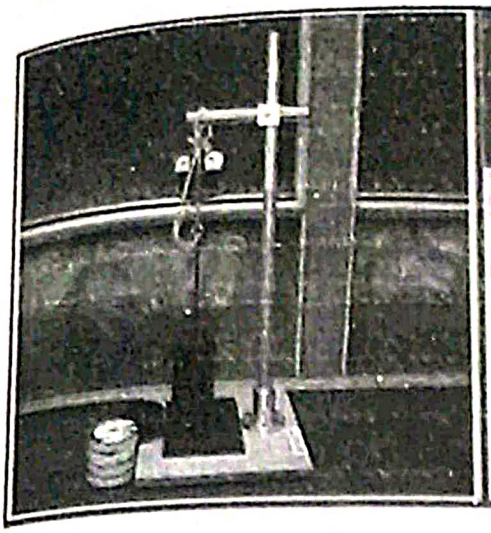
Elementary band theory: Kronig Penny model Band Gap. Conductor, Semiconductor (P and N type) and insulator. Conductivity of Semiconductor, mobility, Hall Effect. Measurement of conductivity (04 probe method) & Hall coefficient.

Superconductivity: Experimental Results. Critical Temperature, Critical magnetic field. Meissner effect. Type I and type II Superconductors, London's Equation and Penetration Depth. Isotope effect. Idea of BCS theory (No derivation)

UNIT – III

6. *ELEMENTARY BAND THEORY*

7. *SUPER CONDUCTIVITY*



Chapter 6

ELEMENTARY BAND THEORY

Bohr's atomic theory explains that in an atom, electrons have well defined energy levels. However, in a crystal an atom gets influenced by large number of neighbouring atoms. Because of this, electrons in the outermost shells of the atoms are forced to have different energies from the energies of electrons in isolated atoms. In solids, the energy levels of outer shells of atoms gets modified. These modified levels are closely confined in a very small energy range. Such a set of closely spaced energy level with continuous energy variation is known as Energy Band. There are three types of energy bands – valence band, forbidden gap band and the conduction band. The highest energy occupied by the valence electrons is called the valence band and the next allowed band is called the conduction band. The band between valence band and conduction band, where no allowed energy level can exist is the forbidden gap. The width of a band depends upon the strength of interaction. A band constitutes energy continuum, in which separate energy levels due to individual atoms cannot be identified. The inner shell electrons are least affected due to interatomic interactions. The electrons present in the valence band have a tendency to conduct and are mostly affected.

In this chapter, we shall study the difference between a conductor, semiconductor and an insulator on the basis of band gap. We will also be studying how conductivity is obtained in semiconductor and will learn the methods to measure the conductivity of semiconductors.

6.1 PERIODIC POTENTIAL IN A CRYSTAL

The graph between the potential energy U of an electron and distance r from the nucleus is shown in Fig. 6.1 and the expression is given as

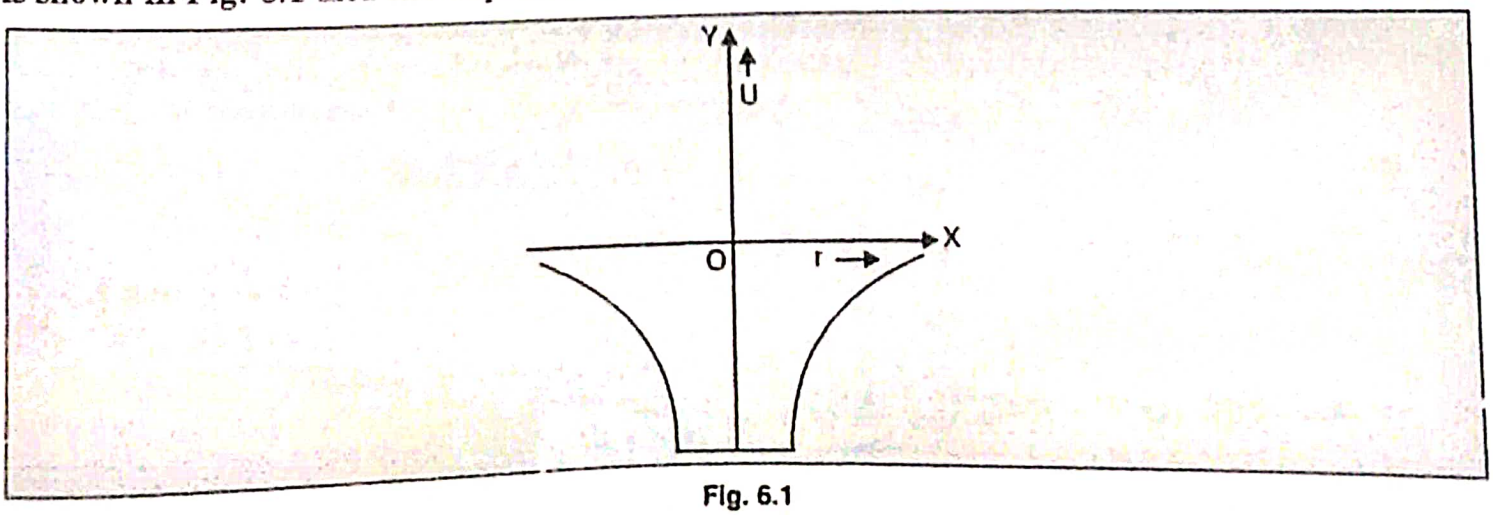


Fig. 6.1

$$U = -\frac{kq^2}{r}$$

where q is the charge and k is constant of proportionality which is equal to $\frac{1}{4\pi \epsilon_0}$. The variations of potential energy with distance in one dimensional case is shown in Fig. 6.2.

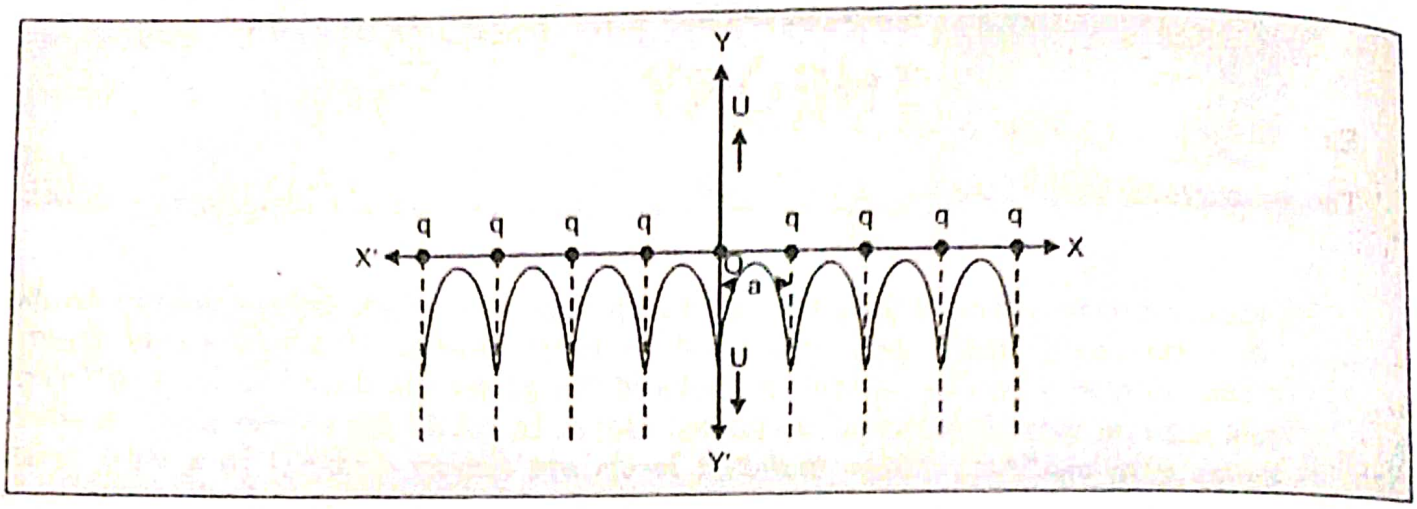


Fig. 6.2

The nucleus in the atom has a positive charge and the electrostatic potential energy of an electron in the field of positive charge is attractive *i.e.* negative as shown in Fig. 6.2. The nucleus is assumed to be at rest and the electron in the crystal is vibrating in a periodic motion with a time period equal to lattice constant a.

Bloch Theorem : When an electron moves with a constant potential V, the Schrodinger wave equation for a time independent one dimensional case is given by

$$\frac{d^2\psi}{dx^2} + \frac{2m}{h^2}(E - V)\psi = 0 \qquad ...(i)$$

The solution of the above equations gives the wave function $\psi(x)$ as

$$\psi(x) = e^{\pm ikx}$$

where $$k = \sqrt{\frac{2m}{h^2}(E - V)}$$

or $$(E - V) = \frac{h^2k^2}{2m}$$

$$= \frac{h^2}{4\pi^2}\frac{4\pi^2}{\lambda^2}\left(\frac{1}{2m}\right) \qquad \left(\because k = \frac{2\pi}{\lambda} \text{ and } h = \frac{h}{2\pi}\right)$$

$$= \frac{h^2}{\lambda^2}\left(\frac{1}{2m}\right)$$

$$= \frac{p^2}{2m} \qquad \left(\because \text{momentum, } p = \frac{h}{\lambda}\right)$$

$$= (\text{K.E.})$$

The physical significance of k is that it is the momentum $\vec{p}$ of the electron divided by h.

$$|\vec{k}| = \frac{2\pi}{\lambda} = 2\pi \frac{mv}{h} = \frac{mv}{\hbar} = \frac{p}{\hbar}$$

Each electron in an atom possesses its own $\vec{k}$ and its own energy.

The solution of the Schrodinger wave equation given in eqn. (*i*) is given by Bloch's theorem or Floquet's theorem which is as follows :

$$\psi(x) = e^{\pm ikx} \mu_k(x) \qquad ...(ii)$$

where $\mu_k(x) = \mu_k(x + a)$ is the wave function due to the periodicity of potential and has period same as that of a lattice. The wave function of the type $\psi(x) = e^{\pm ikx} \mu_k(x)$ is called Bloch function. The Bloch theorem is a mathematical statement regarding the form of the one electron wave functions for a perfectly periodic potential.

6.2 KRONIG-PENNY MODEL

The Kronig Penny model is a simplified model for an electron in a one-dimensional periodic potential. Ralph Kronig (1904 – 1995), a German physicist and William Penny (1909 – 1991) an English mathematician, gave this simple ideal quantum mechanical system which consists of an infinite periodic array of rectangular potential barriers. Before discussing the model let us discuss for energy gap formation.

Reason for energy gap formation : The wave function at the point $k = \pm \frac{\pi}{a}$ do not have travelling waves, instead have stationary waves. When a wave is Bragg reflected, the stationary waves are formed. The resultant wave is time independent and have two different forms of stationary waves in terms of travelling waves $e^{i\pi x/a}$ and $e^{-i\pi x/a}$. These are

$$\psi(+) = e^{i\pi x/a} + e^{-\pi x/a}$$

$$= 2\cos\left(\frac{\pi}{a}\right) \qquad \text{(real part)}$$

and

$$\psi(-) = e^{i\pi x/a} - e^{-i\pi x/a}$$

$$= 2i \sin\left(\frac{\pi x}{a}\right) \qquad \text{(imaginary part)}$$

These two different stationary waves having wave functions $\psi(+)$ and $\psi(-)$ group electrons at different regions with different potential energies. This gives rise to the formation of forbidden gap.

6.4

Earlier Concepts : Prior to Kronig-Penny model, band theory was used to explain the fundamental nature of insulators, conductors and semiconductors. Then, free electron theory helped in explaining the movement of electrons in metals. According to this theory, the valence electrons in a metal absorbs thermal energy which gets converted into kinetic energy with an average of $\frac{3}{2} k_B T$ as per the principle of equipartition of energy. The equipartition principle and the classical Maxwell-Boltzmann's statistics are not sufficient for determining the specific heat of solids. Even magnetic moments of electron due to spin motion could not be explained using the earlier concepts. Later on, the quantum free-electron theory given by Bloch was successful in giving the solution for the Schrodinger equation, in which the wave function includes both a plane wave e^{ikx} which is modulated by the periodic function $\mu_k(x)$ and the state of motion of electron, represented by the wave vector $\vec{k}$. However, the solutions for the Schrodinger's equation with sinusoidal periodicity could not be obtained using Bloch's concept. Hence, Kronig and Penny gave a model in which the inner potential of the crystal system has the rectangular shaped potential.

The Model : In the Kronig-Penny model, a periodic repetition of the potential well as shown in Fig. 6.3 is taken for the calculations. The periodic arrangement of potential wells and barriers is taken for one dimensional case.

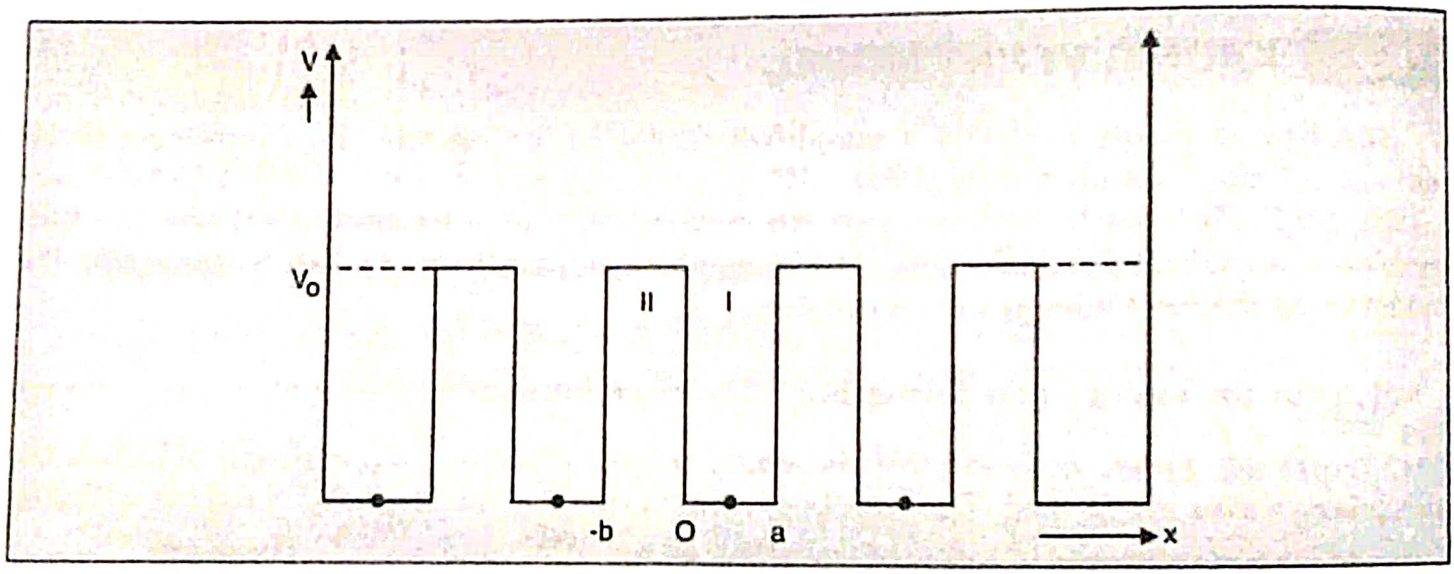


Fig. 6.3

The wave functions linked with this model can be calculated by solving Schrodinger equations for the two regions I and II.

The time independent Schrodinger wave equations for the two regions are

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E)\,\psi = 0 \qquad \text{for } 0 < x < a$$

Putting $\hbar = \frac{2\pi}{h}$, we have,

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi = 0 \qquad \text{for } 0 < x < a \quad ...(i)$$

and $\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E - V_0)\psi = 0$ for $-b < x < a$ ...(ii)

Using Bloch's theorem, we have the solution as

$$\psi(x) = e^{ikx}\mu_k(x)$$

We can define two real quantities α and β, if we assume that the total energy E of the electron is less than the potential energy V_0, then

$$\alpha^2 = \frac{8\pi^2 mE}{h^2}$$

and $$\beta^2 = \frac{8\pi^2 m}{h^2}(V_0 - E)$$

Thus, $\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0$, for $0 < x < a$ ...(iii)

and $\frac{d^2\psi}{dx^2} - \beta^2\psi = 0$, for $-b < x < 0$ ...(iv)

The appropriate solution for region I and region II as per Bloch's theorem is,

$$\psi(x) = \mu_k(x)\, e^{ikx} \quad ...(v)$$

Differentiating the above equation with respect to x, we get

$$\frac{d\psi}{dx} = e^{ikx}\frac{d\mu_k}{dx} + \mu_k ike^{ikx}$$

Differentiating again, we have

$$\frac{d^2\psi}{dx^2} = e^{ikx}\frac{d^2\mu_k}{dx^2} + ike^{ikx}\frac{d\mu_k}{dx} + ike^{ikx}\frac{d\mu_k}{dx} - k^2e^{ikx}\mu_k$$

$$= -k^2e^{ikx}\mu_k + 2ike^{ikx}\frac{d\mu_k}{dx} + e^{ikx}\frac{d^2\mu_k}{dx^2}$$

Substituting the values of $\psi(x)$, $\frac{d^2\psi}{dx^2}$, α^2 and β^2 we have,

$$\frac{d^2\mu_1}{dx^2} + 2ik\frac{d\mu_1}{dx} + (\alpha^2 - k^2)\mu_1 = 0 \quad \text{for } 0 < x < a \quad ...(vi)$$

and $\frac{d^2\mu_2}{dx^2} + 2ik\frac{d\mu_2}{dx} - (\beta^2 + k^2)\mu_2^2 = 0$ for $-b < x < 0$ ...(vii)

where μ_1 represents the value of $\mu_1(x)$ in the interval $0 < x < a$ and μ_2 the value of $\mu_2(x)$ in the interval $-b < x < 0$.

The solution of the equation (*vi*) is of the form,

$$\mu_1 = e^{mx}$$

$$\frac{d\mu_1}{dx} = me^{mx} \quad \text{and} \quad \frac{d\mu_1}{dx^2} = m^2 e^{mx}$$

Substituting these values in eqn. (*vi*), we have

$$m^2 e^{mx} + 2ike^{mx} + (\alpha^2 - k^2)\, e^{mx} = 0$$

$$m^2 + 2ikm + (\alpha^2 - k^2) = 0 \ldots (viii)$$

The solution for m in eqn. (*viii*) is

$$m = \frac{-2ik \pm \sqrt{-4k^2 - 4(\alpha^2 - k^2)}}{2}$$

$$m = -ik \pm i\alpha$$

i.e. $m_1 = i(\alpha - k)$

and $m_2 = -ik - i\alpha$

$= -i\,(\alpha + k)$

Hence, the general solution is

$$\mu_1 = Ae^{m_1 x} + Be^{m_2 x}$$

$$\mu_1 = Ae^{i(\alpha - k)x} + Be^{-i(\alpha + k)x}$$

where A and B are constants.

Similarly, equation (*vii*) can be rewritten as

$$m^2 + 2ikm - (\beta^2 + k^2) = 0 \qquad \ldots (ix)$$

The solution for m in eqa. (*ix*) is

$$m = \frac{-2ik \pm \sqrt{-4k^2 + 4(\beta^2 + k^2)}}{2}$$

$$m = -ik \pm i\beta$$

i.e. $m_1 = -ik + \beta$

$= (\beta - ik)$

and $m_2 = -ik + \beta$

$= (\beta - ik)$

Hence,

$$\mu_2 = Ce^{m_1 x} + De^{m_2 x}$$

or $$\mu_2 = Ce^{(\beta - ik)x} + De^{-(\beta + ik)x}$$

where C and D are constants.

To obtain the values of constants A, B, C and D, we apply boundary conditions

$$\mu_{k_1}(0) = \mu_{k_2}(0) \text{ and } \mu_{k_1}(a) = \mu_{k_2}(-b)$$

$$\left(\frac{d\mu_1}{dx}\right)_{x=0} = \left(\frac{d\mu_2}{dx}\right)_{x=0} \text{ and } \left[\frac{d\mu_1}{dx}\right]_{x=a} = \left(\frac{d\mu_2}{dx}\right)_{x=-b}$$

On applying the boundary conditions, we have,

$$A + B = C + D \qquad \ldots(x)$$

and $\left[Ai(\alpha - k)e^{i(\alpha - k)x} - Bi(\alpha + k)e^{-i(\alpha + k)x}\right]_{x=0}$

$$= \left[C(\beta - ik)e^{(\beta - ik)x} - D(\beta + ik)e^{-(\beta + ik)x}\right]_{x=0}$$

$$i.e.\ i(\alpha - k)A - i(\alpha + k)B = (\beta - ik)C - (\beta + 1k)D \qquad \ldots(xi)$$

And, $Ae^{i(\alpha - k)a} + Be^{-i(\alpha + k)a} = Ce^{-(\beta - ik)b} + De^{(\beta + ik)b}$

$$[Ai(\alpha - k)e^{i(\alpha - k)x} - Bi(\alpha + k)e^{-i(\alpha + k)x}]_{x=a}$$

$$= [C(\beta - ik)x - D(\beta + ik)e^{-(\beta + ik)x}]_{x=-b}$$

or $Ai(\alpha - k)e^{i(\alpha - ik)x} - Bi(\alpha + k)e^{-i(\alpha + k)a}$

$$= C(\beta - ik)b - D(\beta + ik)e^{-(\beta + ik)b}$$

Above equations will have non-zero solutions if the determinant of the coefficients A, B, C and D vanishes. The determinant given below is equal to zero, *i.e.*

$$\begin{vmatrix} 1 & 1 & 1 & 1 \\ i(\alpha - k) & -i(k - \alpha) & (\beta - ik) & -(\beta - ik) \\ e^{i(\alpha - k)a} & e^{-i(\alpha + k)a} & e^{-(\beta - ik)b} & e^{(\beta + ik)b} \\ i(\alpha - k)e^{i(\alpha - k)a} & -i(\alpha - k)e^{-i(\alpha + k)a} & (\beta - ik)e^{(\beta + ik)b} & -(\beta - ik)e^{(\beta + ik)b} \end{vmatrix} = 0$$

On solving we get,

$$\frac{\alpha^2 + \beta^2}{2\alpha\beta}\sinh(\beta b)\sin(\alpha a) + \cosh(\beta b)\cos(\alpha a) = \cos k(a + b)$$

Kronig and Penny assumed that potential energy is zero at lattice sites and equal to V_0 in between them. To make calculations easier, in the above equation, they further assumed that the potential is to be like Dirac delta function *i.e.* $V_0 \longrightarrow \infty$, $b \longrightarrow 0$ and V_0 separated by 'a', so that the quantity $V_0 b$, called barrier strength remains finite.

If $b \longrightarrow 0$, then $\sinh(\beta b) \longrightarrow \beta b$ and $\cosh(\beta b) \longrightarrow 1$

Also, $$\alpha^2 + \beta^2 = \frac{8\pi^2 m}{h^2}V_0.$$

Substituting the value of $(\alpha^2 + \beta^2)$ we have

$$\left(\frac{8\pi^2 m V_0}{2\alpha\beta h^2}\right)\beta b \sin(\alpha a) + \cos \alpha a = \cos ka$$

or $$\frac{P \sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos ka$$

where $$P = \frac{8\pi^2 m V_0 ab}{2\alpha h^2}$$ is a term

which is called the **Scattering power** of the potential barrier. The physical significance of the scattering power is that it is a measure of the strength which electrons in a crystal are attracted to the positive charge of nucleus on the crystal lattice sites. Putting $\frac{h}{2\pi} = \hbar$, we can write P as

$$P = \frac{m V_0 ab}{\hbar^2}$$

In simple words, we can say that the scattering power P is a measure of potential barrier. Higher is the value of P, more strong will be the binding of the electrons in a particular potential well.

Since $$-1 \leq \cos ka \leq 1$$

hence, $$-1 \leq \frac{P \sin(\alpha a)}{\alpha a} + \cos(\alpha a) \leq 1$$

Therefore all values of (αa) are not allowed. As all sine and cosine functions vary from – 1 to + 1, so only those values of (αa) are allowed for which the term $\frac{P \sin \alpha a}{\alpha a} + \cos \alpha a$ has to take values between + 1 and – 1. This can be shown in the Fig. 6.4.

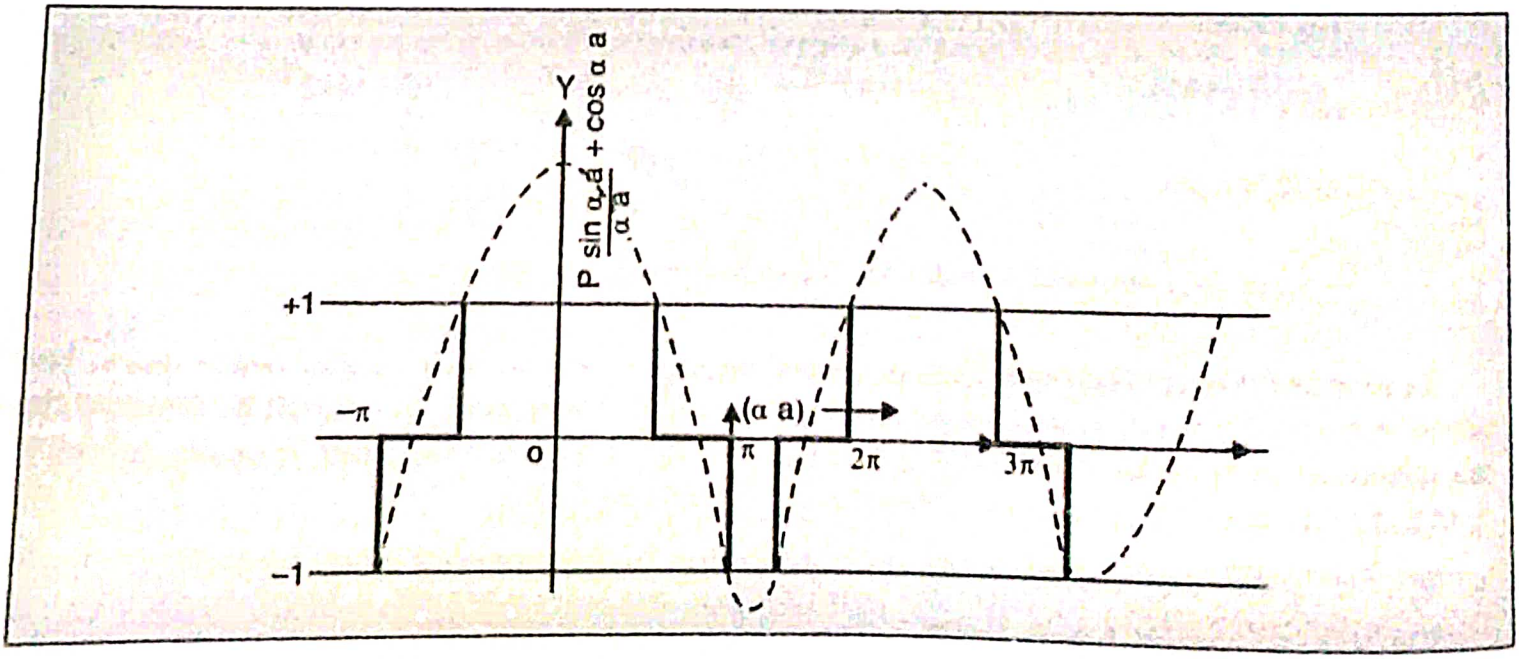


Fig. 6.4

6.3 CONCLUSIONS OF KRONIG-PENNY MODEL

(*i*) The energy spectrum of electron in the periodic lattice consists of allowed and forbidden bands. The allowed bands are shown in thick dark lines separated by intervals where there are no energy levels in Fig. 6.4. The boundaries of the allowed bands corresponds to the values of cos $(ka) = \pm 1$.

$$ka = n\pi$$

or

$$k = \frac{n\pi}{a}$$

or

Thus, the wave number should be an integral multiple of $\frac{\pi}{a}$.

(*ii*) As the product (αa) increases, the scattering power P decreases. Subsequently, the width of allowed energy bands increases and thus the forbidden energy bands become narrower.

(*iii*) When scattering power P tends to infinity, then, the allowed energy bands become infinitely narrow. Thus, when $P \to \infty$, then,

$$\sin \alpha a = 0$$

or

$$\alpha a = \pm n\pi$$

or

$$\alpha^2 = \frac{n^2\pi^2}{a^2}$$

Hence

$$E = \frac{\alpha^2\hbar^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

The above expression for E opines that E is independent of wave number k. The discrete energy spectrum is same as that of particle in one dimensional potential well of side a. The effect of changing P on the energy band structure is shown in Fig. 6.5.

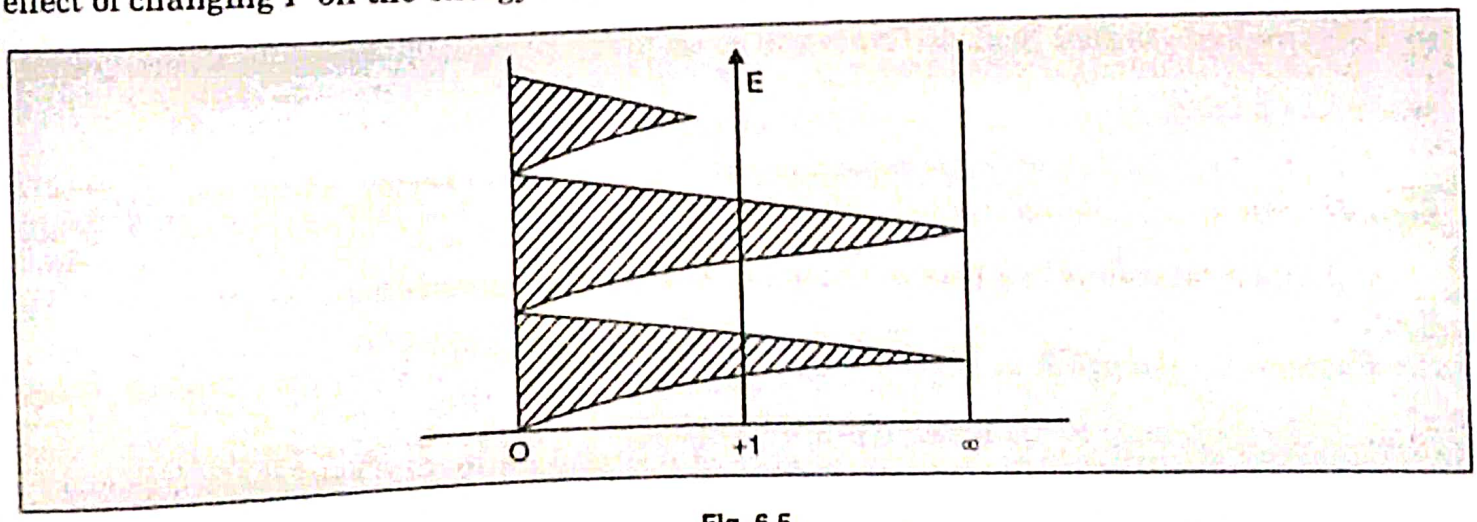


Fig. 6.5

The allowed range is shown in shaded portion whereas the forbidden energy states are shown in open portion in Fig. 6.5. The extreme left represents $P = 0$ whereas the extreme right corresponds to $P = \infty$.

The energy spectrum is quasi-continuous for $P = 0$.

The energy spectrum is a line spectrum for $P = \infty$. In between P = 0 and $P = \infty$, the position and width of the allowed and forbidden band is represented by drawing a vertical line as shown in Fig. 6.6 which plots a graph between E along Y-axes and k along X-axes.

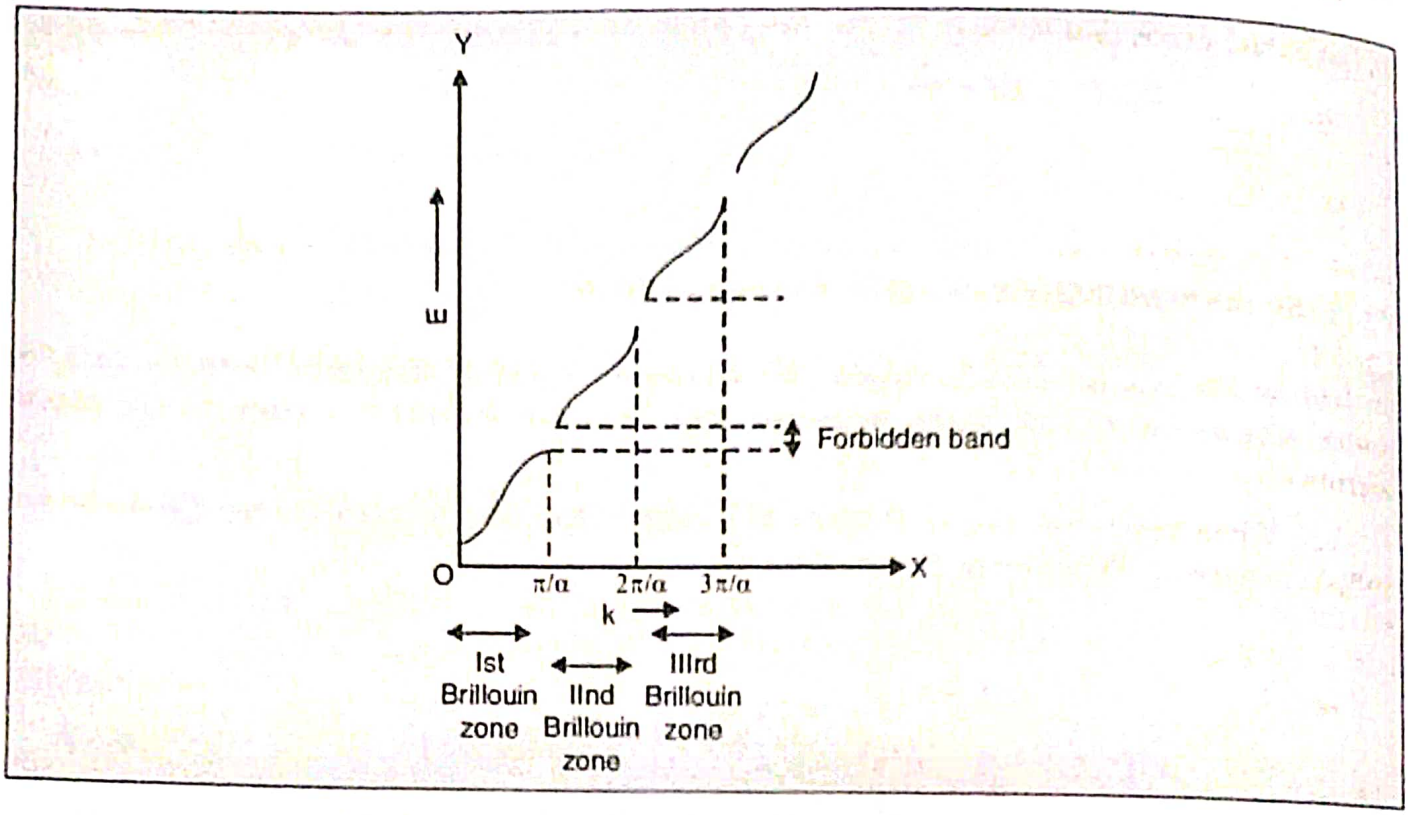


Fig. 6.6

(*iv*) In the graph E versus k in Fig. 6.6, discontinuities takes place at $k = \frac{\pi}{a}, \frac{2\pi}{a}, \frac{3\pi}{a}, \ldots\ldots, \frac{n\pi}{a}$ where n is an integer, (*i.e.* $n = 1, 2, 3, \ldots\ldots$). The k-values given us first, second, third etc. Brillouin zones. For $k = \frac{\pi}{a}$ to $\frac{-\pi}{a}$, we have first Brillouin zone. From $\frac{+\pi}{a}$ to $\frac{+2\pi}{a}$ we have second Brillouin zone and so on. Each portion of the curve in the Fig. 6.6 is termed as a band.

(*v*) The boundaries of zone represents the maximum energies which an electron can possess without any discontinuity.

(*vi*) The total energy is a periodic function of k, within a given energy band.

Suppose we change k to $k + \frac{2\pi n}{a}$ then the equation $\frac{P \sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$ remains same. This is because of the mathematical fact that

$$\cos\left(k + \frac{2\pi n}{a}\right) a = \cos (ka + 2n\pi) = \cos (ka)$$

(*vii*) As per de Broglie's theory, wave packet is associated with moving electron and the group velocity v_g of the wave packet is same as that of velocity of electron

$$v = v_g = \frac{d\omega}{dk}$$

We also know that the energy associated with electron is

$$E = \hbar\omega$$

Hence, the velocity $\vec{v} = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{dE}{dk}$

$$= \frac{1}{\hbar} \text{ (slope of } E \text{ versus } k \text{ graph)}$$

The changes in the energy corresponding to wave vector $\vec{k}$ of electrons in Kronig-Penny model is shown in Fig. 6.7. The slope of $E - k$ curve in the graph at the top and bottom is, so the velocity of electron at the top and bottom is also zero. The slope is maximum at $k = k_0$, therefore the velocity of electron is also maximum at $k = k_0$. The point where the slope of E versus k graph is maximum is known as point of inflexion.

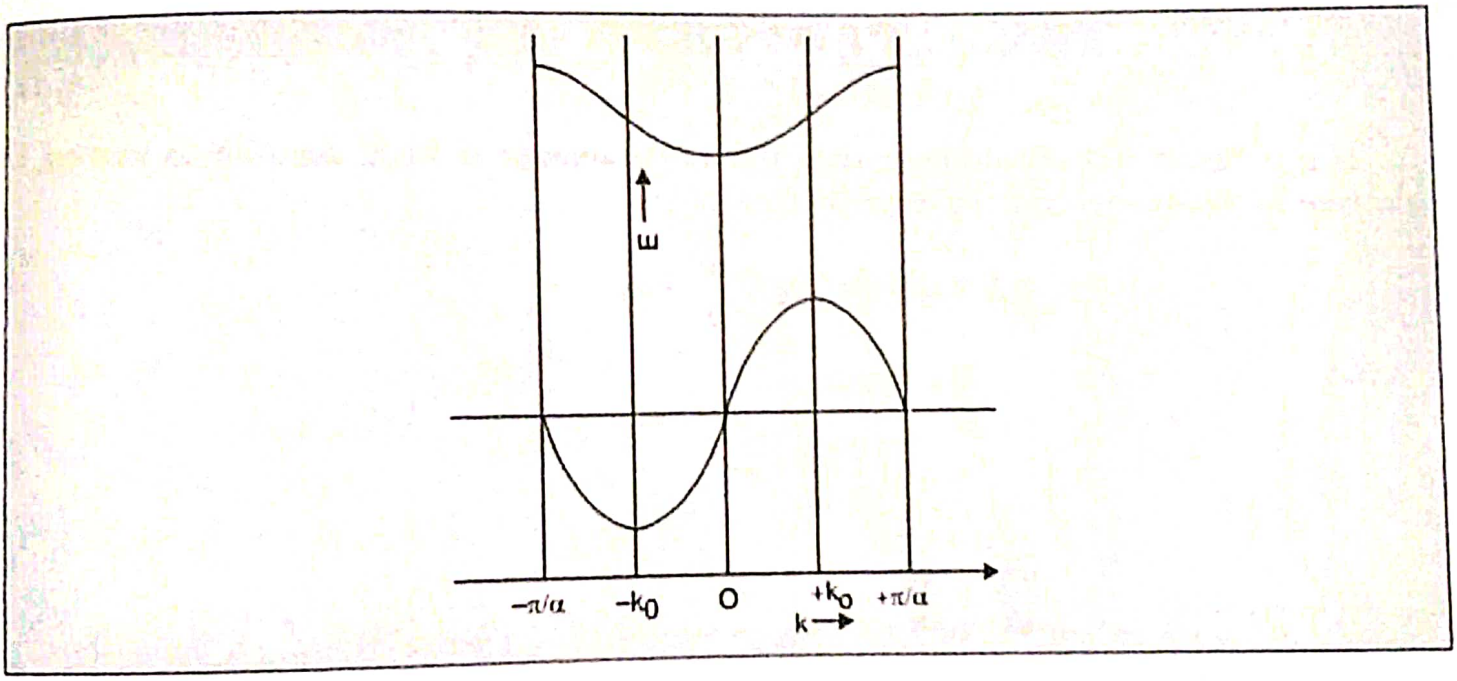


Fig. 6.7

When electron is free, then there is no energy band and the energy corresponding to free electron is expressed as

$$E = \frac{\hbar^2 k^2}{2m}$$

Hence $\vec{v} = \frac{1}{\hbar}\frac{dE}{dk} = \frac{\hbar k}{m} = \frac{p}{m}$

If we plot a graph between velocity of electron and wave vector $\vec{k}$, then the graph indicates that velocity increases linearly with $\vec{k}$ (Fig. 6.8).

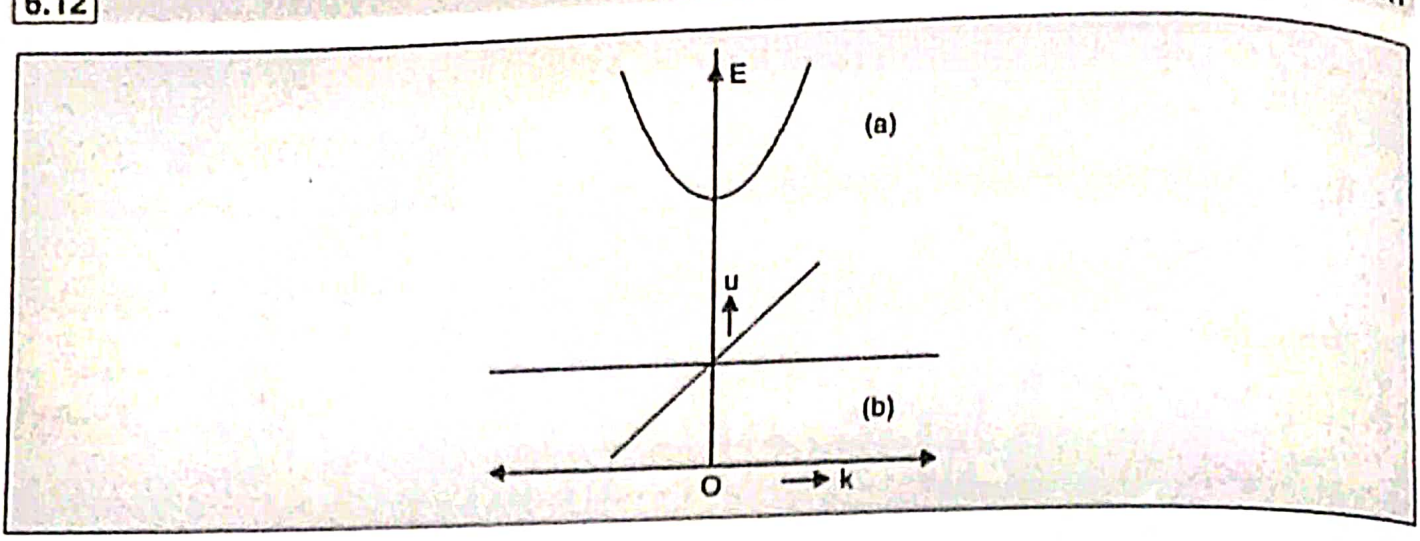


Fig. 6.8

(*vii*) The acceleration of the electron moving in an external electric field ξ is given by

$$a = \frac{d}{dt}(v) \text{ where } v \text{ is the velocity of electron.}$$

$$= \frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{dk}{dt} \qquad \left(\because v = \frac{1}{\hbar}\frac{dE}{dk}\right)$$

If q is the charge on electron, then the small amount of work done dE in moving the electron by displacement dx by external force $q\xi$ is

$$dE = (q\xi)\,dx = (q\xi)\,\frac{dx}{dt} \times dt$$

$$= q\,\xi\,v_g\,dt$$

$$= q\,\xi\left(\frac{1}{\hbar}\frac{dE}{dk}\right)dt$$

or $$\frac{dk}{dt} = \frac{q\xi}{\hbar}$$

Hence, acceleration $a = \dfrac{q\xi}{\hbar^2}\dfrac{d^2E}{dk^2}$

or $$q\xi = \left[\frac{\hbar^2}{(d^2E/dk^2)}\right]a$$

The effective mass (m_{eff}) of vibrating electron in the crystal is

$$m_{eff} = \frac{\hbar^2}{d^2E/dk^2} \qquad \left(\because \frac{q\xi}{a} = \text{mass}\right)$$

Point to Remember

Effective mass of electron in a crystal is in inversely proportional to d^2E/dk^2.

The graph between kinetic energy E with respect to wave vector $\vec{k}$ is shown in Fig. 6.9.

At $$k = \pm \frac{\pi}{a},\ E \text{ is maximum}$$

$$\therefore \quad \frac{d^2E}{dk^2} = -ve$$

At $k = k_0$, the slope of E versus k graph is maximum,

$$\therefore \quad \frac{d^2E}{dk^2} = 0$$

Therefore, in the region between $\left(-\frac{\pi}{a}\right)$ to $-k_0$ and between k_0 to $\left(\frac{+\pi}{a}\right)$, the value of $\frac{d^2E}{dk^2}$ is negative

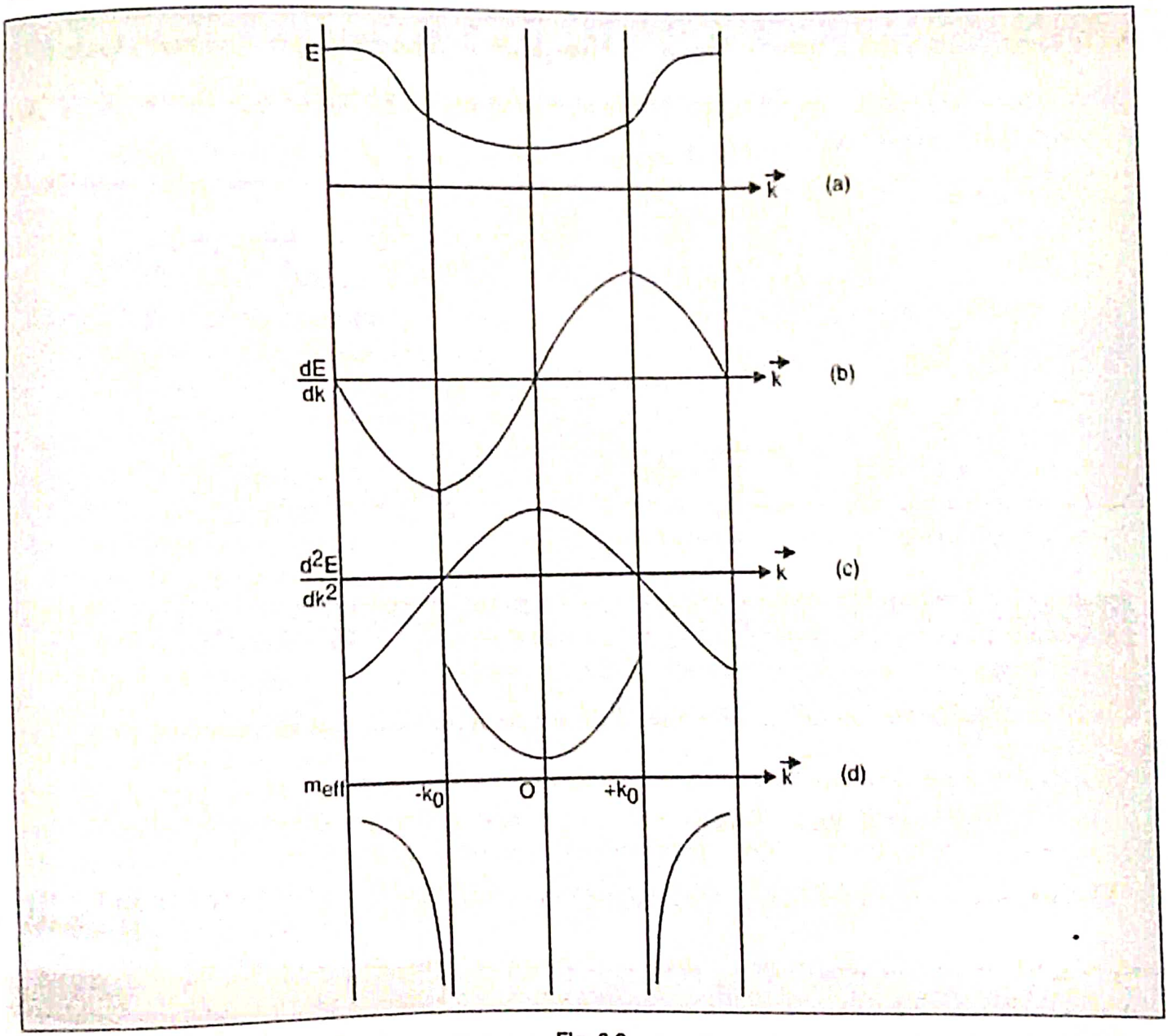


Fig. 6.9

(viii) When the effective mass is greater than the normal mass of the electron, then the electron is being bounded with lattice. The effective mass will be more if the binding is strong.

When effective mass is infinite at $k = \pm k_0$, it means that at given value of k, the electron is strongly bounded with lattice. The negative value signifies Bragg's reflection at Brillouin zone boundaries.

6.4 BAND GAP : CONDUCTORS, SEMICONDUCTORS AND INSULATORS

Let us calculate the effective number of free electrons in a band so as to differentiate between conductors, insulators and semiconductors on the basis of band gap. We know that the electron in k-state is actually bounded to a lattice and therefore the effective mass of the electron is different from free electron mass.

Let us consider an empty band which is filled with electrons upto wave vector k_1 within the first Brillouin zone shown in Fig. 6.10. Here $k_1 < \frac{\pi}{a}$. The ratio of free electron mass to its effective mass in k-state can be taken as the extent to which an electron in that k state is free to take part in conduction.

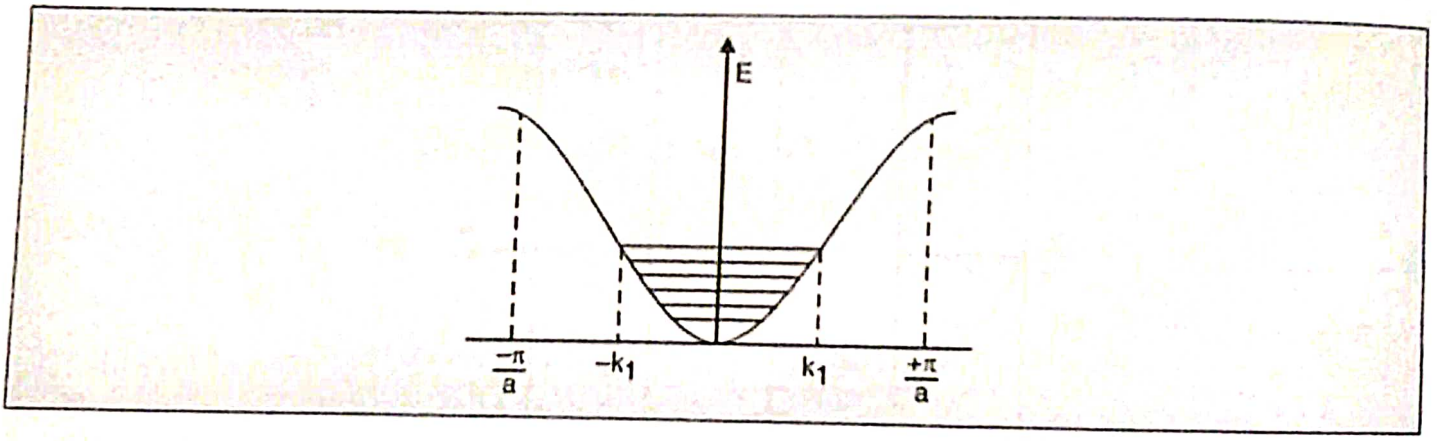


Fig. 6.10

i.e.
$$f_k = \frac{m}{m_{eff}} = \frac{m}{\hbar^2}\frac{d^2E}{dk^2}$$

Now in one dimension lattice of length L, the number of states in the interval dk is given by

$$dn = \frac{L}{2\pi}dk$$

Therefore, the effective number of electrons in interval dk is,

$$dN_{eff} = 2f_k \frac{L}{2\pi}dk$$

The factor 2 is due to Pauli's exclusion principle which states that each state is filled by

two electrons. Hence, integrating dN_{eff}, we get the total number of effective electrons if the band is filled upto k_1 is

$$N_{eff} = 2 \int_{-k_1}^{+k_1} f_k \frac{L}{\pi} dk = \frac{2Lm}{\pi\hbar^2} \left(\frac{dE}{dk}\right)_{k = k_1}$$

Hence, the effective number of electrons available for conduction depends on the (dE/dk).

Band Gap : The difference between the highest value of energy in a given band and the lowest value of energy in the very next band above it is called the band gap. Band gaps are also called forbidden energy states.

The allowed energy bands in a solid at lowest temperature *i.e.* $0K$, lowest energy are filled with the available electrons from the bottom upwards, as per Pauli's exclusion principle, till all the electrons are accommodated. With the increase of temperature, the electrons in the valence band shift to still higher empty levels in the conduction band. The application of electric field or magnetic field also compels the electrons to cross the band gap and shift to conduction band. All solids do not behave alike. So some solids are classified conductors, some insulators and some are referred as semiconductors.

For a completely filled band, for example at the first Brillouin zone boundaries, $k = \pm \frac{\pi}{a}$, the slope of the curve in Fig. 6.10 is zero, as the graph is flat at the top.

So when $\frac{dE}{dk} = 0$, then $N_{eff} = 0$.

This means that the number of free electrons in a completely filled band is zero. The point at which the band is filled upto $k = k_0$ is called inflexion point. At this point the effective number of electrons becomes maximum.

Insulators are those solids where there are no free electrons. All energy bands are completely full in the valence band and the conduction band is entirely vacant. In insulators, there is a large forbidden energy gap between valence band and conduction band. It is practically impossible to excite any electron across the forbidden band as the band gap energy for insulators is approximately more than 6 eV [Fig. 6.11(a)].

Point to Remember

At inflexion point, the nature of slope, in the graph between E and k, changes sign from positive to negative.

Even if an external electric field is applied to an insulator or temperature of insulator is raised, no current is produced as all the bands are then either completely filled or empty. Hence the conductivity of insulators under ordinary conditions is zero. As an example, diamond is a material whose covalent bond splits $2s$ and $2p$ levels into two band separated by an energy gap of $\Delta E_g = 7\ eV$ with the valence electrons filling the lower band and so diamond is an insulator.

In fig. 6.11 (*d*), there is no energy gap with $E_g = 0\ eV$, now it is easy for electrons to be available for conduction. On the application of external field in any form such as electric, heat etc., electrons shifts from valence band to the conduction band, so these type of solids are called conductors. Even if there is a small energy gap as shown in fig. 6.11 (c), materials such

as *Li*, *Na*, *K* etc. exhibit the conductivity. In the case of materials such as *Ba*, *Cd*, *Zn* etc. the valence band is completely filled and the empty conduction band overlaps the valence band. The electrons freely move inside the crystal lattice and cause conduction.

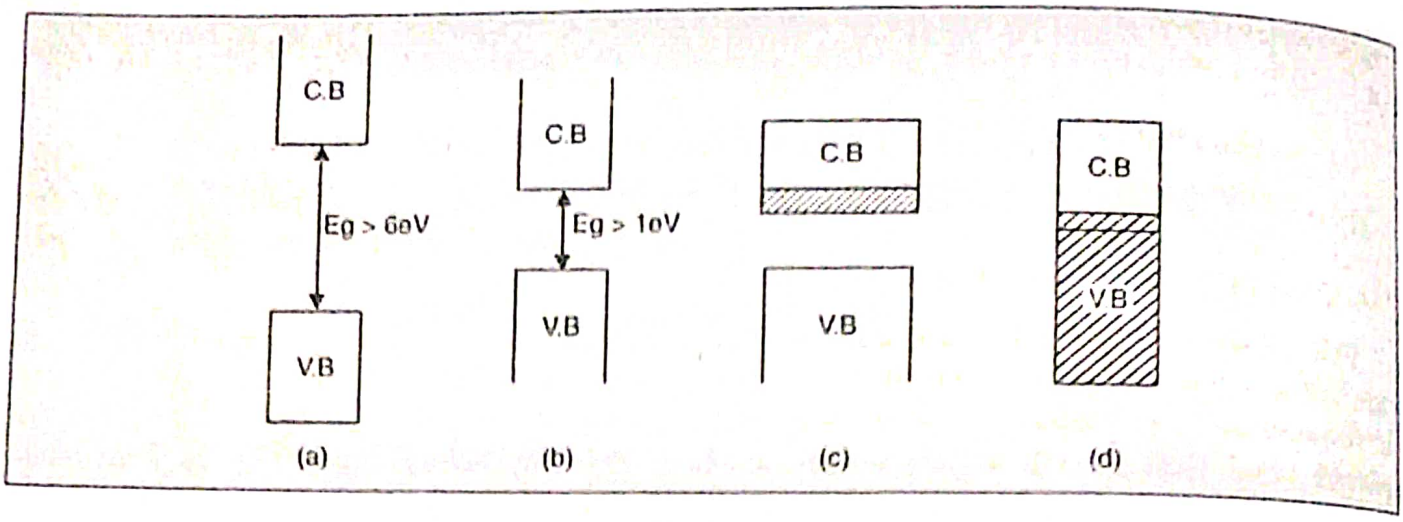


Fig. 6.11

Semiconductors are those solids where the band gap energy is very small of the order of 1 *eV* which can be overcome by the application of external electric field or raising the temperature. At a temperature close to zero Kelvin, the valence band is completely filled and the conduction band is fully empty. At this temperature semiconductor behaves as an insulator.

Conclusions :

(i) If the valence electrons exactly fill one or more bands, leaving other empty, the crystal is an insulator [Fig. 6.11(*a*)].

(ii) If the bands overlap, then instead of one filled band and the other over it fully empty, giving an insulator, we can have two partly filled bands giving a metal.

(iii) If the energy gap is very small ($E_g \simeq 0.025$ *eV*) at room temperature, the electrons can rise from valence band to the conduction band on the application of field. Band overlap with some gap as in Fig. 6.11 (*c*), the crystals are called semi metals. Bismuth is an example of semi-metal.

6.5 SEMICONDUCTORS (P AND N TYPE)

A pure semiconductor in which no impurity is added is called intrinsic conductor. The conductivity of a pure semiconductor depends upon the number of electrons excited from valence band to conduction band. Semiconductors can be in the form of elements on their compounds. Examples of elemental semiconductors are Germanium (*Ge*) and Silicon (*Si*) whereas inorganic compounds such as *CdS*, *GaAs*, *GaP*, *CdSe* and *InP* are some examples of compound semiconductors. The total current (I) in a semiconductor is the sum of current flowing due to electrons (I_e) and the current flowing due to holes (I_h) *i.e.* $I = I_e + I_h$.

Point to Remember

All semiconductors have crystalline structure.

Limitations of Intrinsic Semiconductor

(i) In an intrinsic semiconductor, the number of intrinsic charge carriers at room temperature is very small ($\approx 10^{16}$ per m^3).

Point to Remember

Ge is obtained from ash of coals and from flue dust of zinc smelters.

(ii) The breakage of covalent bonds due to thermal motion is the only cause of production of intrinsic charge carriers. Therefore it is difficult to control their number in intrinsic semiconductors.

(iii) The number of electrons are equal to the number of holes in intrinsic semiconductors. Hence, we cannot have large number of only electrons or holes in intrinsic semiconductors.

Extrinsic Semiconductor : A semiconductor doped with suitable impurity is called extrinsic semiconductor. These are of two types :

(i) *N*-type semiconductor

(ii) *P*-type semiconductor

Point to Remember

Silicon is found in most of the common rocks. Sand is silicon dioxide from which silicon is extracted.

N-type Semiconductor : If pentavalent impurity atoms such as arsenic, antimony, phosphorus, bismuth etc. are doped to an intrinsic (pure) semiconductor, *N*-type semiconductor is obtained. Only four out of five available electrons of impurity atoms participate in forming the covalent bonds and fifth electron from each impurity atom is almost free for conduction as shown in Fig. 6.12. When a fifth group element substitutes the sites of *Si* or *Ge*, then pentavalent dopant donates one extra electron for conduction and hence is called donar impurity. Total number of conduction electrons (n_e) is due to the contribution of donars as well as thermally generated carriers. But the number of holes (n_h) are only due to thermal process. In this type of semiconductors since the majority charge carriers are negatively charged electrons, so this type of semiconductor is *N*-type semiconductor.

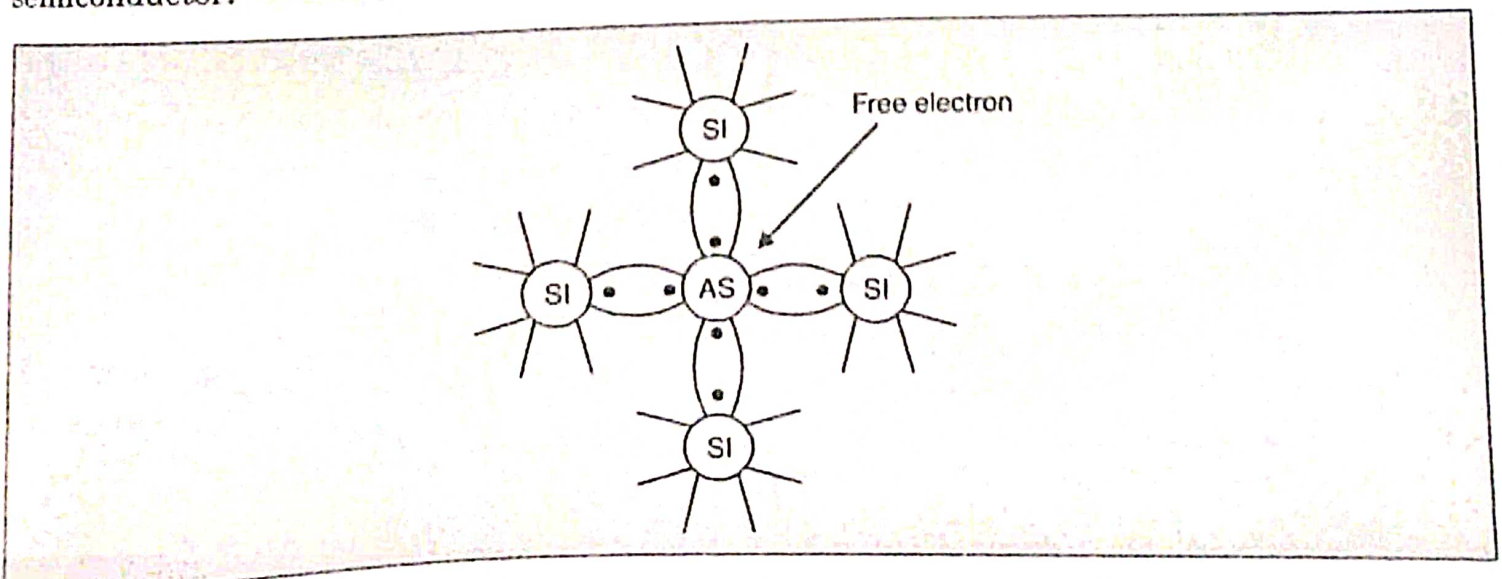


Fig. 6.12

There is a very little attraction between the fifth free electron and core of the impurity atom. Very small part of energy, less than 0.045 eV, is required to make the electron move from valence band to conduction band. The thermal energy at room temperature is enough to make the fifth electron free for the conduction. Fifth group impurity atoms are called donar atoms as they donate the electrons for conduction.

When fifth group impurity atoms are added to an intrinsic semiconductors, then energy possessed by the free electrons, due to impurity atoms, is slightly less than the energy of free electrons in the lowest energy level of the conduction band. These electrons create a lower energy level just below (0.01 eV to 0.05 eV) the conduction band as shown in Fig. 6.13. This energy band is called donar energy level. Since the energy gap reduces due to creation of donar energy level, electrons can easily go to the conduction band, even at room temperature. Thus the conductivity of N-type semiconductors increases greatly.

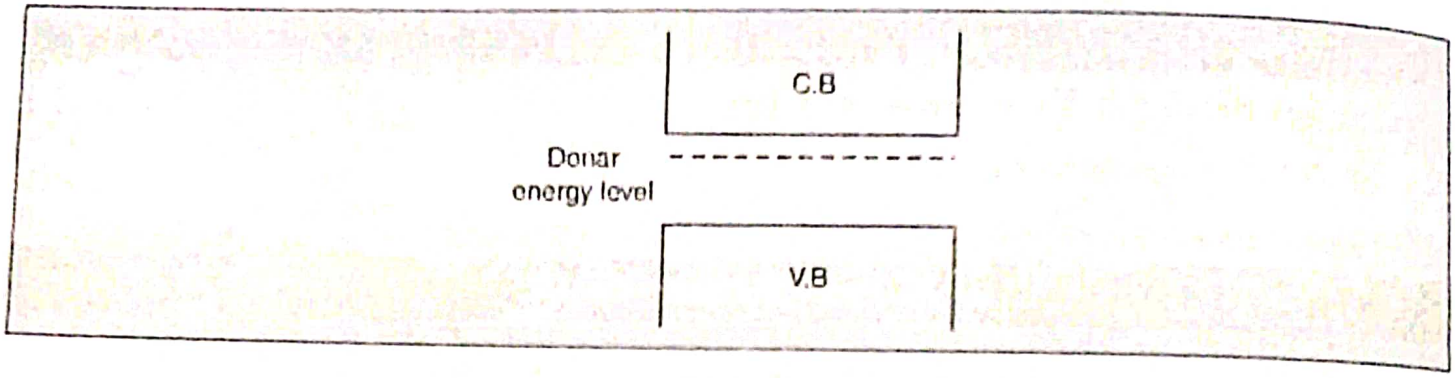


Fig. 6.13

P-Type Semiconductor : If trivalent atoms such as Boron, Aluminium, Gallium, indium etc. are doped to an intrinsic semiconductor, P-type semiconductor is obtained. Trivalent impurity atoms form only three covalent bonds with the neighbouring semiconductor atoms. One covalent bond remains incomplete due to the deficiency of electron as shown in Fig. 6.14. To fill this incomplete bond, an electron is taken from a neighbouring *Si-Si* bond, which creates a vacancy or a hole there. To fill this hole, another covalent bond in the neighborhood gets broken and in this way holes are the majority current carriers and the semiconductor produced is called a P-type semiconductor as holes carry positive charge. These holes which move freely in a crystal lattice cause conductivity. Trivalent impurity atoms are called **acceptors** because they accept electrons from the neighbourhood bonds.

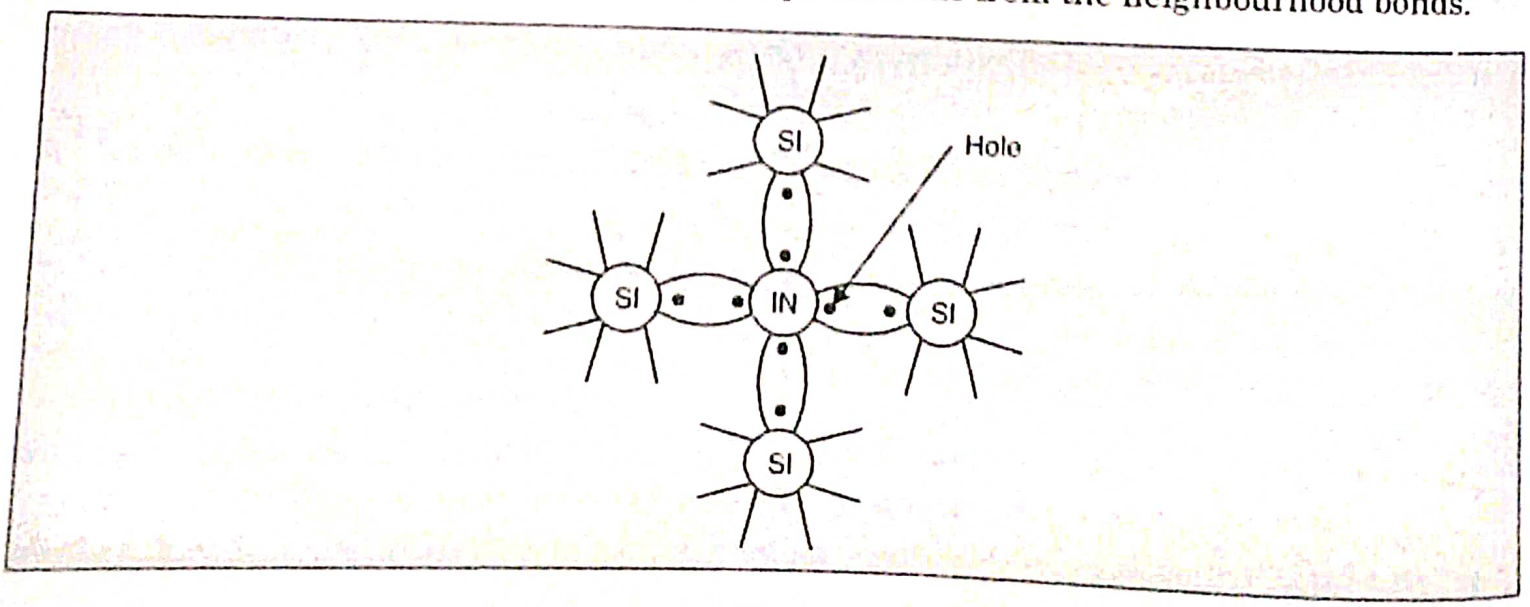


Fig. 6.14

The holes create a acceptor energy level just above the top of the valence bond. At room temperature, the electrons get sufficient thermal energy and can jump easily from the valence band to the acceptor energy level and creates further holes in the valence band as shown in Fig. 6.15.

Density of electrons in C.B. of N-Type Semiconductor : Let us calculate the density of electrons in conduction band and density of holes in valence band of N-type extrinsic semiconductor.

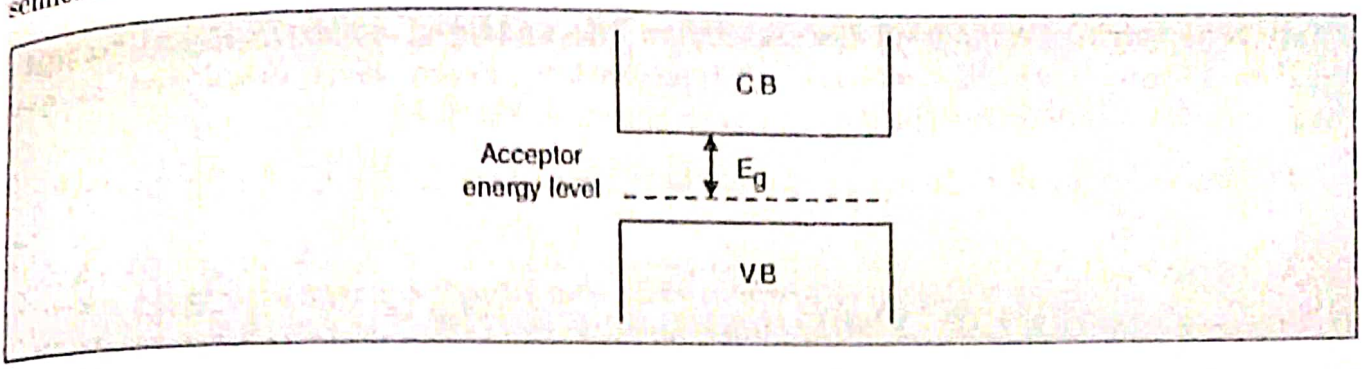


Fig. 6.15

We know that the number of electrons (n_e) per unit volume in conduction band is given by the relation

$$n_e = N_{eff}\, e^{\frac{E_F - E_C}{k_B T}} \qquad \ldots(i)$$

where E_C is the energy corresponding to the bottom of conduction band, N_{eff} is the total number of effective electrons in the band and is given by

$$N_{eff} = \frac{2LM}{\pi\hbar^2}\left(\frac{dE}{dk}\right)_{k = k_1}$$

E_F is the energy corresponding to a fermi level, k_B is the Boltzman's constant and T is the temperature. Also, the number of vacant states per unit volume in donar level shown in Fig. 6.13 is

$$= N_d\, e^{E_d - E_F/k_B T} \qquad \ldots(ii)$$

Comparing eqns. (i) and (ii) we have,

$$N_{eff}\, e^{\frac{E_F - E_C}{k_B T}} = N_d\, e^{\frac{(E_d - E_F)}{k_B T}}$$

or
$$\frac{N_d}{N_{eff}} = e^{\frac{2E_F - E_d - E_C}{k_B T}}$$

$$\log_e\left(\frac{N_d}{N_{eff}}\right) = \frac{2E_F - E_d - E_C}{k_B T}$$

$$= \frac{2E_F}{k_B T} - \frac{(E_d + E_c)}{k_B T}$$

or $$E_F = \frac{E_d + E_c}{2} + \frac{k_B T}{2} \log_e \left(\frac{N_d}{N_{eff}} \right) \quad \ldots(iii)$$

At $T = 0K$,

$$E_F = \frac{E_d + E_c}{2}$$

At zero kelvin, Fermi level lies exactly in the middle of donar level and bottom of conduction band with the increase of temperature, Fermi level drops and at room temperature, it comes below the donar level as shown in Fig. 6.16.

Putting the value of E_F from eqn. (*iii*) in eqn. (*i*), we have

$$n_e = N_{eff}\, e^{\left[\frac{E_d - E_c}{2k_B T} + \frac{1}{2} \log_e \frac{N_d}{N_{eff}} \right]} = N_{eff} \left[e^{\frac{E_d - E_c}{2k_B T}} \right] \left[\frac{N_d}{N_{eff}} \right]^{1/2}$$

$$= \sqrt{N_{eff} N_d} \left[e^{\frac{E_d - E_c}{2k_B T}} \right] = \sqrt{N_{eff} N_d}\; e^{\frac{\Delta E}{2k_B T}}$$

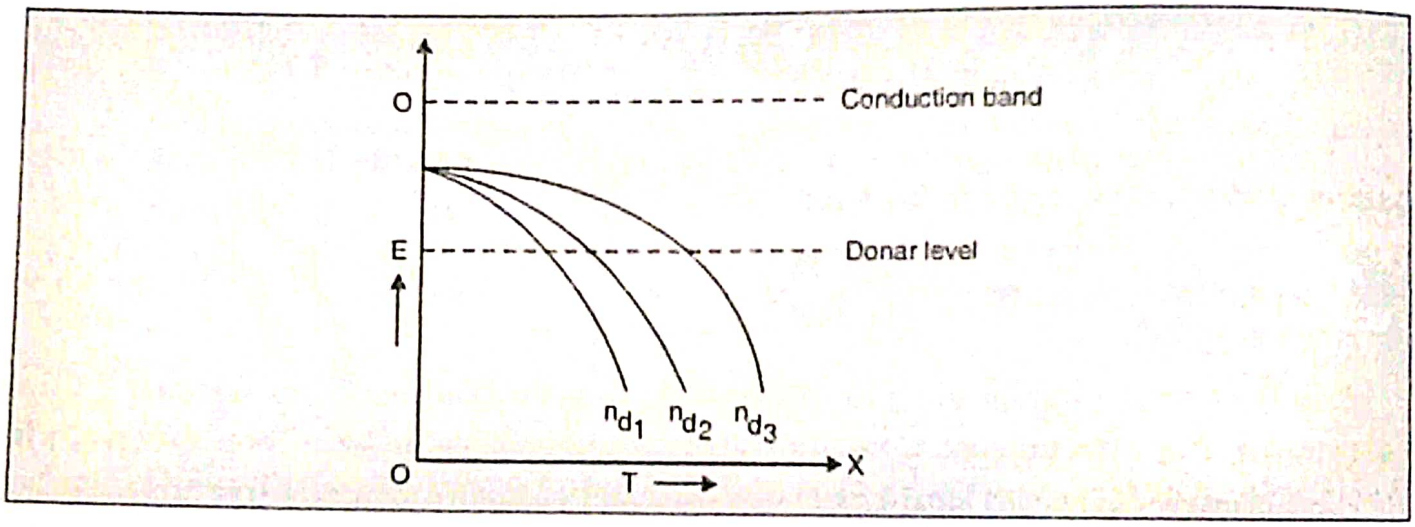


Fig. 6.16

where $\Delta E = E_d - E_c$ is the ionization energy of donar impurity.

Thus, we conclude that

(i) The density of electrons in the conduction band is proportional to the square root of the donar concentration.

(ii) The conductivity of intrinsic semiconductor is less than *N*-type or *P*-type semiconductor.

(iii) There is a limit on the operating temperature of semiconductor materials.

(iv) Similarly the carrier concentration of holes in the valence band of *P*-type semiconductor can be determined as

$$n_h = \sqrt{N_{eff} N_a}\; e^{\Delta E / 2k_B T}$$

where N_a is the number of acceptor atoms per unit volume. Here, the Fermi level lies exactly midway between top of valence band and acceptor level (Fig. 6.15). With increase in temperature, it shifts upwards.

6.6 CONDUCTIVITY AND MOBILITY OF SEMI CONDUCTORS

Consider a semiconductor of length l, area of cross-section A in which n_e number of electrons and n_p number of holes flow when a potential difference V is applied. The total current I is given by

$$I = I_e + I_h$$

where I_e, the current due to flow of electrons is given by

$$I_e = n_e A e v_e$$

Here, e is the electric charge and v_e is the drift velocity of electrons. Similarly, if v_h is the drift velocity of holes, then

$$I_h = n_p e A v_h$$

Hence, $$I = n_e e A v_e + n_h e A v_h$$

or $$\frac{I}{A} = n_e e v_e + n_h e v_h$$

or $$J = e (n_e v_e + n_h v_h)$$

where $J = \frac{I}{A}$ is the current density.

In terms of conductivity, J is the product of electrical conductivity σ and electric field intensity E. Therefore,

$$\sigma E = e (n_e v_e + n_h v_h)$$

or $$\sigma = \frac{n_e e v_e}{E} + \frac{n_h e v_h}{E}$$

$$= n_e e \mu_e + n_h e \mu_h$$

where μ_e and μ_h are the mobilities of electrons and holes.

The mobility of electrons μ_e is greater than the mobility of holes. Thus $I_e > I_h$.

The electrical conductivity of N-type semiconductor is determined by using the relation

$$\sigma_N = N_d e \mu_e$$

where N_d is the number of donar impurity atoms per unit volume.

Temperature dependence of electrical conductivity : Starting from temperature of zero kelvin to 10 K, the conductivity increases with rise in temperature. This rise is due to the increase in the number of conduction electrons due to ionisation of donars in N-type semiconductor. The conductivity becomes maximum when all donars are ionised.

The graph between $\log_e \sigma$ and $1/T$ is shown in Fig. 6.17. From point B in the graph, the conductivity decreases with further rise in temperature upto point C. This is because of decrease in the mobility μ_e with increase in temperature. After point C, the conductivity increases sharply till point D.

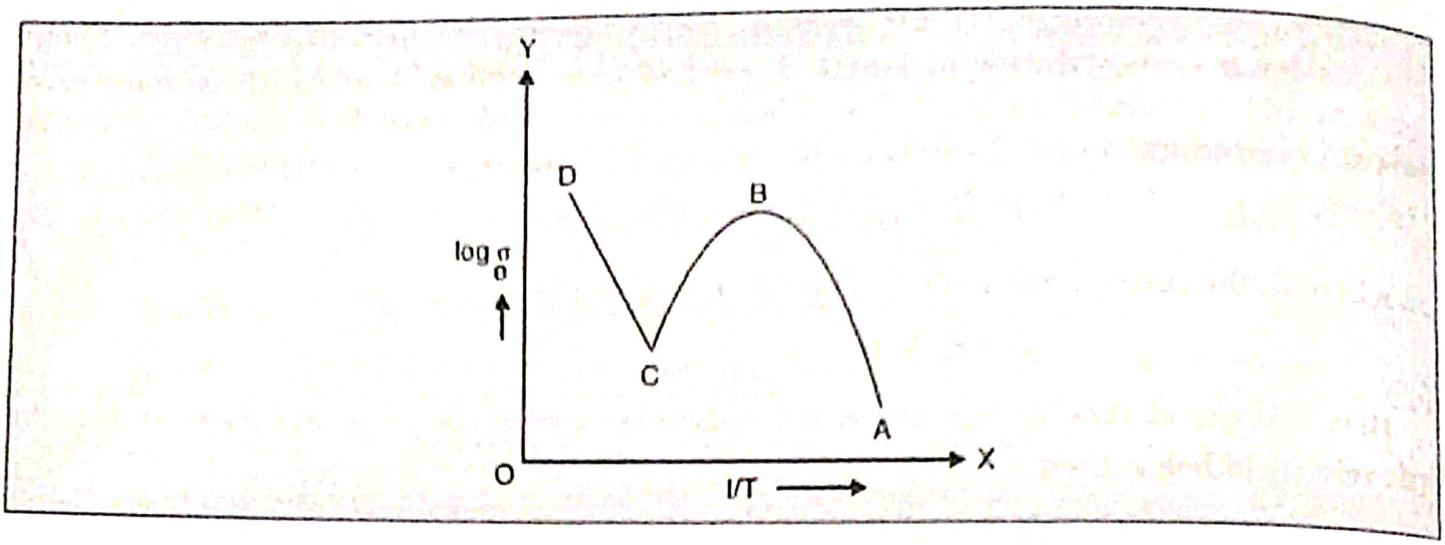


Fig. 6.17

The electrical conductivity of a P-type semiconductor is given by

$$\sigma_P = N_A e \mu_h$$

where N_A is the number of acceptor impurity atoms. The variation of conductivity with changes in temperature is similar to that for N-type semiconductor

6.7 HALL EFFECT

Hall-Effect in semiconductors comes from motion of both electrons and holes. Edwin Hall (1855 – 1938) an American physicist in 1879 explained this effect which states that **"when a current carrying conductor is placed in a magnetic field mutually perpendicular to the direction of current, a potential difference is developed at right angles to both the magnetic and electric field."**

Hall Effect in Semiconductors : When a current carrying semiconductor is placed in a magnetic field, the charge carriers of the semiconductor experience a force in a direction perpendicular to both the magnetic field and the current.

Hall effect gives the best experimental proof of the motion of holes.

Hall Electric field (E_y) : Let us derive an expression for the Hall electric field E_y when both electrons and holes are deflected transversely with an applied electric field E_x along X-axis and a transverse component of magnetic field B_z is applied along Z-axis.

The electron current density J_{xe} along x-axis is given as

$$J_{xe} = n_e \mu_e E_x$$

where n_e is the number of electrons and μ_e is the mobility of electrons.

Similarly, the expression for hole current. The net transverse current density J_y along Y-axis is density along x-axis is given by

$$J_{xh} = n_p \mu_p E_x$$

where n_p is the number of holes and μ_p is the mobility of holes.

The total current density J_x along X-axis in a semiconductor is given as

$$J = J_{xe} + J_{xh}$$

$$= e (n_e \mu_e + n_h \mu_h) E_x$$

Now, the magnetic Lorentz force acting on an electron moving with drift velocity v_e in the magnetic field B_z is equal to $-e (v_e \times \vec{B}_z)$ or is equal to $e v_y B_z$. This Lorentz force is equivalent to an electric field $- v_e B_z$. We know that the drift velocity $\vec{v}_e = \mu_e \vec{E}_x$ and therefore,

$$J_{ye} = n_e e \mu_{ez} (\mu_e B_z E_x)$$

$$= n_e e^2 \mu_e^2 B_z E_x$$

Similarly hole current density along y-axis is

$$J_{yh} = n_h e \mu_h^2 B_z E_x$$

$$J_y = J_{ye} + J_{yh}$$

$$= e (n_e \mu_e^2 - n_h \mu_h^2) B_z E_x$$

To make net current along y-axis equal to zero, a Hall electric field E_y is required.

The ratio $$\frac{E_y}{E_x} = \frac{J_y}{J_x}$$

$$\therefore \quad e(n_e \mu_e + n_h \mu_h) E_y = - e (n_e \mu_e^2 - n_p \mu_h^2) B_z E_x$$

or $$- E_y = \left[\frac{n_h \mu_h^2 - n_e \mu_e^2}{n_e \mu_e + n_h \mu_h}\right] B_z E_x$$

6.8 MEASUREMENT OF CONDUCTIVITY AND HALL COEFFICIENT

The Hall Coefficient R_H is defined as the ratio of the electric field induced to the product of the current density J_x and the applied magnetic field Bz. Mathematically

$$R_H = \frac{E_y}{B_Z J_x} = \frac{n_h \mu_h^2 - n_e \mu_e^2}{e (n_e \mu_e + n_h \mu_h)^2}$$

Four Probe Method : This is a simple method in which a rectangular shaped semiconductor in the form of a wafer is taken. It consists of four probes arranged linearly in a straight line at equal distances from each other. A constant current is passed through the two probes and the potential difference is measured across the middle two probes.

Experimental Setup : A rectangular specimen of a semiconductor of width b and thickness t is placed between the pole pieces of an electromagnet as shown in Fig. 6.17.

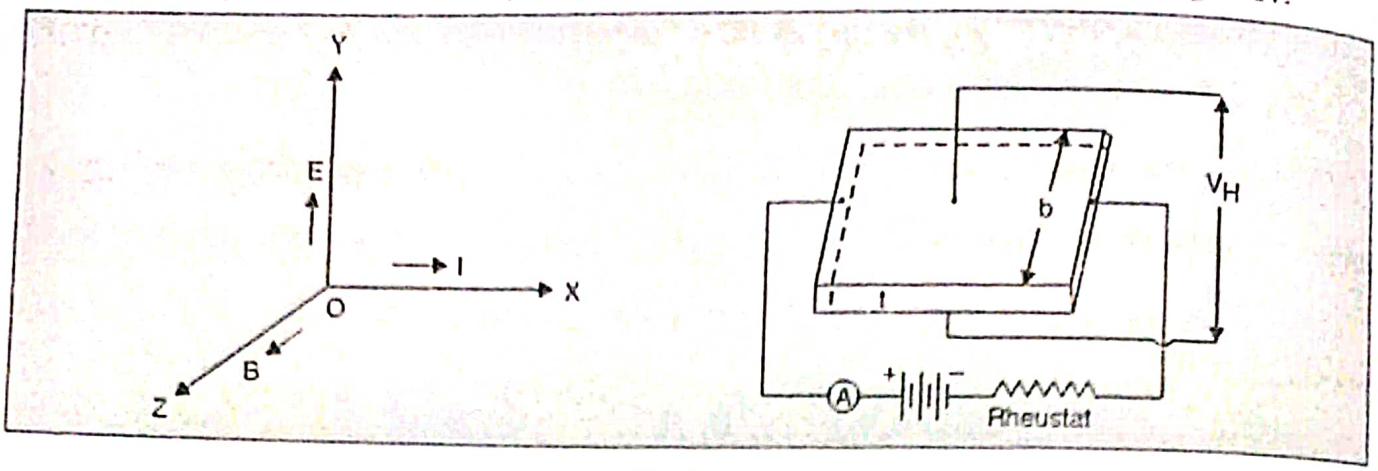


Fig. 6.17

A magnetic field $\vec{B}$ is applied along the Z-axis perpendicular to the applied electric field. A current I passes along X-axis from a battery. An ammeter A is connected in series to measure the current.

Calculations : The Hall voltage V_H is measured by placing two probes at the centre of the bottom and top surfaces of semiconductor sample (Fig. 6.17).

$$V_H = E_H t$$

where Hall electric field $E_H = R_H J B_Z$

So that

$$V_H = R_H J B_Z t$$

Now, we know that the current density J is given as

$$J = \frac{I}{\text{Area}}$$

$$= \frac{I}{tb} \qquad (\because \text{Area} = \text{thickness} \times \text{breadth})$$

we know that $J = \sigma E_H$

or conductivity, $\sigma = = \frac{J}{E_H} = \frac{I}{\tau b E_H}$

and $R_H = \frac{V_H\, b}{I\, B_Z}$

S.I. unit of Hall coefficient R_H is m^3/Coulomb.

USES : (i) Determination of semiconductor type can be obtained if the Hall coefficient is positive, then it a P-type semiconductor. For negative value of R_H, we have N-type semiconductor.

(*ii*) By measuring Hall coefficient R_H, we can find electron concentration n_e and hole concentration n_p.

(*iii*) Using this method, by measuring the conductivity σ and Hall coefficient, we can measure the mobility μ.

(*iv*) We can also measure the strength of magnetic field B by knowing the Hall voltage, Hall coefficient and amount of current passed.

(*v*) This method can be used to determine the power flow in an electromagnetic wave. This is done by knowing that the Hall voltage is proportional to the product of $\vec{E}$ and $\vec{\beta}$.

SOLVED PROBLEMS

PROBLEM 1. **An insulator has an optical absorption which occurs for all wavelengths lesser than 1400 Å. Find the width of the forbidden energy band for the insulator.**

Solution

Here wavelength $\lambda = 1400$ Å

$= 1400 \times 10^{-10}\ m$

Corresponding frequency $f = \dfrac{c}{\lambda}$

$= \dfrac{3 \times 10^8}{1400 \times 10^{-10}}$

Hence, the energy gap $E_g = hf$

$= \dfrac{6.626 \times 10^{-34} \times 3 \times 10^8}{1400 \times 10^{-10}}$

$= 1.41 \times 10^{-18}\ J$

$= \dfrac{1.41 \times 10^{-18}}{1.6 \times 10^{-19}} = 8.81$ eV

PROBLEM 2. **Determine the concentration of conduction electrons per (metre)^3 in intrinsic semiconductor whose conductivity is $3 \times 10^4\ \Omega\ m^{-1}$. Electron and hole mobilities are 0.14 and 0.06 m^2/Vs respectively.**

Solution

Here $\sigma_e = 3 \times 10^4 \Omega^{-1}\ m^{-1}$

$\mu_e = 0.14\ m^2/Vs$

$$\mu_h = 0.06\ m^2/Vs$$

$$n_e = ?$$

Using the relation we have,

$$\sigma_e = n_e\, e\, \mu_e + n_p\, e\, \mu_h$$

For intrinsic semiconductors, $n_e = n_p$

$$\therefore \qquad \sigma_e = n_e\, e\, (\mu_e + \mu_h)$$

Substituting the values we have

$$3 \times 10^4 = n_e \times 1.6 \times 10^{-19}\,[0.14 + 0.06]$$

$$n_e = \frac{3 \times 10^4}{1.6 \times 10^{-19} \times 0.20} = \mathbf{9.37 \times 10^{23}}$$

PROBLEM 3. **The Fermi level in certain semi-conducting material is 1 75 eV at a particular temperature. Calculate the number of free electrons per unit volume in the semiconductor at the same temperature. Given the lattice parameter a = $\frac{\pi}{3}$.**

Solution

Here,Fermi energy E_F= 1.75 eV

$$= 1.75 \times 1.6 \times 10^{-19}$$

$$= 2.8 \times 10^{-19}\ J$$

lattice parameter a= $\frac{\pi}{3}$

mass of electron m= 9.1×10^{-31} kg

Use the relation

$$E_F = \frac{n^2 \pi^2 h^2}{2\, m\, a^2}$$

Putting $h = \frac{h}{2\pi}$, we get

$$E_F = \frac{n^2\, h^2}{8\, m\, a^2}$$

or $$n^2 = \frac{8\, m\, E_F\, a^2}{h^2}$$

or $$n = \sqrt{\frac{8\, m\, E_F}{h^2}}\, a$$

$$= \left[\frac{8 \times 9.11 \times 10^{-31} \times 2.8 \times 10^{-19}}{(6.62 \times 10^{-34})^2}\right]^{1/2} \times \frac{\pi}{3}$$

$$= 2.15 \times 10^{18} \times \frac{\pi}{3}$$

$$= 2.25 \times 10^{18} \text{ electrons per } m^3$$

PROBLEM 4. **Calculate the concentration of electrons and holes in N type semiconductor if the donar density is 10^{22} atom/m^3 and the intrinsic carrier concentration is 1.5×10^{20} per m^3 at room temperature.**

Solution

Here, the number density of donars $N_d = 10^{22}$ atom/m^3

Number of intrinsic carriers $n_i = 1.5 \times 10^{20}/m^3$

We know that $n_e n_p = n_i^2$

Here $n_e = N_d$

or $$n_p = \frac{n_i^2}{N_d}$$

$$= \frac{(1.5 \times 10^{20})^2}{10^{22}} = 2.25 \times 10^{18} \text{ atoms/m}^3$$

PROBLEM 5. **The energy near the valence band edge of the crystal is given by $E = -Ak^3$ where $A = 10^{-36}$ Jm^2. Calculate the effective mass of electron with wave vector having magnitude of 10^9 m^{-1}.**

Solution

Here, $E = -Ak^3$, $k = 10^9$ and $A = 10^{-36}\ Jm^2$

So $$\frac{dE}{dk} = -A(3k^2)$$

and $$\frac{d^2E}{dk_2} = -A(6k)$$

We know that effective mass is given by the relation

$$m_{eff} = \frac{\hbar^2}{\left(\frac{d^2E}{dk^2}\right)} = \frac{\left(\frac{h}{2\pi}\right)^2}{[-6 \times 10^{-36} \times 10^9]}$$

$$= -\frac{(1.053 \times 10^{-34})^2}{6 \times 10^{-45}} = -0.184 \times 10^{-23} \text{ kg}$$

PROBLEM 6. **In an N-type semiconductor, the Fermi level lies 0.35 eV below the conduction band. If the concentration of donar atoms is made three times, then find the new position of Fermi level. Consider k_BT = 0.03 eV.**

Solution

If N_d is the number of donar atoms, E_F and E_c be Fermi level and conduction band level, then

$$N_d = N_{eff}\, e^{(E_F - E_c)/k_BT}$$

Let N_d' be the number of donar atoms after change in concentration when energy corresponding to fermi level is E_F', then

$$N_{d'} = N_{eff}\, e^{(E_F' - E_c)/k_BT}$$

Now, $\dfrac{N_d'}{N_d} = 3$ (given)

and $(E_F - E_c) = 0.35\ eV$

$$\frac{N_d'}{N_d} = \frac{e^{(E_F' - E_c)/k_BT}}{e^{(E_F - E_C)/k_BT}}$$

or $$3 = \frac{\exp\left[(E_F' - E_c)/k_BT\right]}{\exp\left[(E_F - E_c)/k_BT\right]}$$

$$\log_e 3 = \frac{(E_F' - E_c)}{k_BT} - \frac{(E_F - E_c)}{k_BT}$$

$$= \frac{(E_F' - E_c) - (E_F - E_c)}{k_BT}$$

or $(E_F' - E_c) = \log_e 3\,(k_BT) + (E_F - E_c)$

$= 1.0986 \times 0.03 + 0.35$

$= 0.3829$ eV

PROBLEM 7. **A copper strip 2.0 cm in breadth and 0.8 mm thick is placed in a magnetic field of induction 1 Tesla. If a current of 100 A is set up in the strip, how much Hall voltage appears across the strip ? One cubic metre of copper strip contain 8.4×10^{28} electron.**

Solution

Here $I = 100\ A$

$b = 2 \times 10^{-2}\ m$

$t = 0.8 \times 10^{-3}\ m$

Area of cross-section $A = bt$

$= 2.0 \times 10^{-2} \times 0.8 \times 10^{-3}$

$= 1.6 \times 10^{-5}\ m^2$

Magnetic field $B = 1$ Tesla

$n = 8.4 \times 10^{28}\ m^{-3}$

We know that

Hall coefficient $R_H = \dfrac{E_y}{B_Z J_x}$

$= \dfrac{V_y}{b\, J_x\, B_z} = \dfrac{1}{ne}$

or $V_y = \dfrac{b\, I_x\, B_z}{n\, e\, A}$

$= \dfrac{2 \times 10^{-2} \times 100 \times 1}{8.4 \times 10^{28} \times 1.6 \times 10^{-19} \times 1.6 \times 10^{-5}}$

$= 0.093 \times 10^{-4}$ V

PROBLEM 8. **A semi-conducting crystal 1.0 mm long, 5 mm wide and 0.51 mm thick, has a magnetic flux density of 2 Tesla applied from front to back perpendicular to the largest face. When a current of 10 A flows length wise through the specimen, the voltage measured across its width is found to be 30 μV. What is the Hall coefficient of the semiconductor, if a specimen of copper of similar dimensions and with same 10 A current flowing along its length is placed in the same magnetic field. Given number of atom per unit volume equal to 8.5×10^{28} atoms m^{-3}.**

Solution

Here, Hall voltage produced,

$V_H = 30\ \mu V = 30 \times 10^{-6}\ V$

Width, $b = 5\ mm = 5 \times 10^{-3}\ m$

Magnetic field $B_Z = 2$ Tesla

Thickness $t = 0.51\ mm$

$= 0.51 \times 10^{-3}\ m$

Hall coefficient $R_H = \dfrac{E_y}{J_x B_Z}$

$= \dfrac{V_H}{b\, J_x\, B_Z} = \dfrac{1}{nc}$

$$\text{Current density } J_x = \frac{\text{Current } (I)}{\text{area } (bt)}$$

$$= \frac{10}{5 \times 10^{-3} \times 0.51 \times 10^{-3}}$$

$$= 153.78 \times 10^6 \, Am^{-2}$$

$$\text{Hall coefficient } R_H = \frac{30 \times 10^{-6}}{5 \times 10^{-3} \times 0.51 \times 10^{-3} \times 2}$$

$$= 5.88 \, C^{-1} \, m^3$$

If semiconductor is replaced by copper of same dimensions, then

$$R_H = \frac{V_H}{bJ_xB_Z} = \frac{1}{n_e}$$

where n is number of atoms per unit volume.

In terms of density ρ and atomic weight M and Avogadro's number N, we have,

$$n = \frac{N_\rho}{M} = 8.5 \times 10^{28} \, m^{-3} \quad \text{(given)}$$

$$e = 1.6 \times 10^{-19} \, C$$

Thus $$V_y = \frac{b \, J_x B_Z}{ne}$$

$$= \frac{5 \times 10^{-3} \times 153.78 \times 10^6 \times 2}{8.5 \times 10^{28} \times 1.6 \times 10^{-19}}$$

$$= 113.07 \times 10^{-6} \text{ V}$$

CONCEPTUAL QUESTIONS

Q. 1. Give the cause of failure of free electron theory ?

Ans. The free electron theory could not explain the difference between conductors, semiconductors and insulators. The theory could not answer the spherical nature of Fermi surfaces. Even the concepts of Hall coefficients of metals and semiconductors could not be explained by the theory. This is due to the fact that in actual practice the electrons move in a periodic potential whereas the free electron theory assumes that the electrons orbit in a constant potential around the nucleus.

Q. 2. What is the basic assumption given by Kronig and Penny in their theory ?

Ans. Kronig and Penny suggested that the electrons move in a periodic potential such that the potential energy of an electron in a linear array of positive nuclei has the form of a periodic array of square wells.

Q. 3. Plot a graph between kinetic energy and wave vector k of the free electron.

Ans.

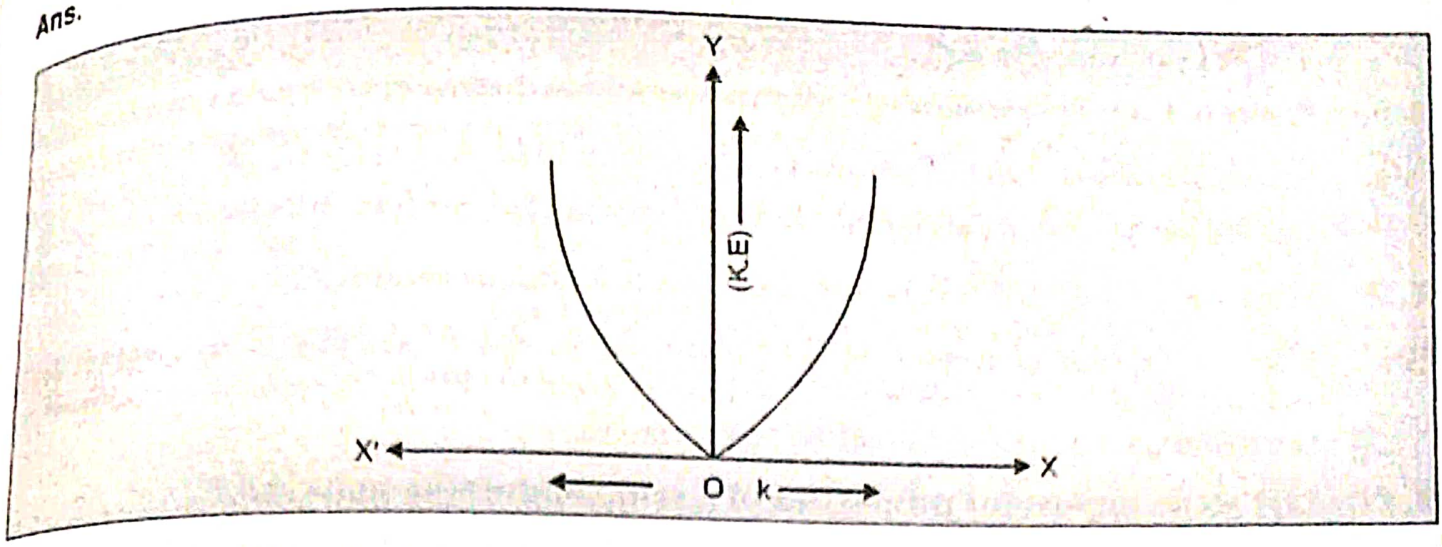


Fig.

Q. 4. When does the velocity of electron become maximum ?

Ans. We know that the velocity (v) of electron is given by the expression

$$\vec{v} = \frac{1}{\hbar}\left(\frac{dE}{dk}\right)$$

It becomes maximum at inflexion points of kinetic energy E versus wave vector $\vec{k}$ curve where it approaches the free electron velocity. The velocity of electron decreases with increase in energy beyond the inflexion point.

Q. 5. Define forbidden energy gap as per Kronig-Penny Model of atom ?

Ans. As per Kronig-Penny model, the energy spectrum of electron consists of a number of allowed energy bands separated by forbidden regions. These forbidden regions are called forbidden gaps.

Q. 6. What are the factors on which the effective mass of electron depends ?

Ans. The effective mass of an electron moving in a crystal depends on the shape of energy versus wave vector k curve. It is expressed as

$$m_{eff} = \hbar^2 \left[\frac{d^2E}{dk^2}\right]^{-1}$$

Q. 7. What is a Fermi surface ?

Ans. A Fermi surface is the surface in K-space inside which all the states are occupied by the valence electrons. All the states lying outside the surface are empty.

Q. 8. What are the symmetry properties which satisfies the concept that kinetic energy is a function of wave vector k ?

Ans. (*i*) Translational symmetry : $E(K + G) = E(K)$

This helps us to confine our considerations to the first Brillouin zone only.

(*ii*) Inverse symmetry : $E(-K) = E(K)$

(*iii*) Rotational symmetry.

Q. 9. What is the value of energy gap in a semiconductor ?

Ans. The approximate value of energy gap in a semiconductor is about 1 eV.

For Silicon $E_g = 1.15\ eV$ and for Ge, it has a value of $0.75\ eV$.

Q. 10. What is an hole ? What is hole current in semiconductors ?

Ans. When a vacancy is created in the valence band due to shifting of an electron from valence band to conduction band, a hole is created. When current is constituted by the movement of holes, it is called hole current.

Q. 11. List some important properties of a semiconducting material ?

Ans. (*i*) Semiconductors have negative temperature coefficient of resistance.

(*ii*) The resistivity of semiconductors changes from 10^{-5} to $10^{4}\ \Omega m$.

(*iii*) The electrical conductivity of semiconductor increases by suitable doping.

(*iv*) Semiconductors have high thermoelectric power with sign both positive and negative relative to a given metal.

Q. 12. What is the charge on P and N type semiconductors ?

Ans. The net charge on P-type and N-type semiconductor is zero. When we add pentavalent impurities in the semiconductor each pentavalent atom gives one free electron and pentavalent atom acquires positive charge and therefore semiconductor remains neutral.

Q. 13. What is Hall Effect ?

Ans. When a current carrying conductor is kept in a magnetic field mutually perpendicular to the direction of current, a potential difference is set up at right angle to both the magnetic field and electric field. This phenomenon is called Hall effect.

Q. 14. What is the cause of Hall-potential ?

Ans. When a current carrying material is placed in a transverse magnetic field, the magnetic field exerts a deflecting force called Lorentz force, in the direction perpendicular to both magnetic field and drift velocity. This causes charges to shift from one surface to another thus creating a potential difference.

Q. 15. Which type of charge has greater mobility ?

Ans. Electrons have greater mobility than hole.

Q. 16. Tin, Carbon, Silicon and Germanium are all group XIV elements. Yet tin is a conductor, carbon is an insulator while Si and Ge are semiconductors. Why ?

Ans. In conductors, there is no band gap between conduction band and valence band. For insulators band gap is large ($\geq 6\ eV$). As band gap for tin is close to $0\ eV$, for carbon it

This helps us to confine our considerations to the first Brillouin zone only.

(*ii*) Inverse symmetry : $E(-K) = E(K)$

(*iii*) Rotational symmetry.

Q. 9. What is the value of energy gap in a semiconductor ?

Ans. The approximate value of energy gap in a semiconductor is about 1 eV.

For Silicon $E_g = 1.15\ eV$ and for Ge, it has a value of $0.75\ eV$.

Q. 10. What is an hole ? What is hole current in semiconductors ?

Ans. When a vacancy is created in the valence band due to shifting of an electron from valence band to conduction band, a hole is created. When current is constituted by the movement of holes, it is called hole current.

Q. 11. List some important properties of a semiconducting material ?

Ans. (*i*) Semiconductors have negative temperature coefficient of resistance.

(*ii*) The resistivity of semiconductors changes from 10^{-5} to $10^{4}\ \Omega m$.

(*iii*) The electrical conductivity of semiconductor increases by suitable doping.

(*iv*) Semiconductors have high thermoelectric power with sign both positive and negative relative to a given metal.

Q. 12. What is the charge on P and N type semiconductors ?

Ans. The net charge on *P*-type and *N*-type semiconductor is zero. When we add pentavalent impurities in the semiconductor each pentavalent atom gives one free electron and pentavalent atom acquires positive charge and therefore semiconductor remains neutral.

Q. 13. What is Hall Effect ?

Ans. When a current carrying conductor is kept in a magnetic field mutually perpendicular to the direction of current, a potential difference is set up at right angle to both the magnetic field and electric field. This phenomenon is called Hall effect.

Q. 14. What is the cause of Hall-potential ?

Ans. When a current carrying material is placed in a transverse magnetic field, the magnetic field exerts a deflecting force called Lorentz force, in the direction perpendicular to both magnetic field and drift velocity. This causes charges to shift from one surface to another thus creating a potential difference.

Q. 15. Which type of charge has greater mobility ?

Ans. Electrons have greater mobility than hole.

Q. 16. Tin, Carbon, Silicon and Germanium are all group XIV elements. Yet tin is a conductor, carbon is an insulator while Si and Ge are semiconductors. Why ?

Ans. In conductors, there is no band gap between conduction band and valence band. For insulators band gap is large ($\geq 6\ eV$). As band gap for tin is close to $0\ eV$, for carbon it

is 5.4 eV, for Si it is 1.1 eV and for Ge it is 0.75 eV, therefore, tin is a good conductor, carbon is close to insulator whereas Ge and Si are semiconductors.

Q. 17. Derive an expression for mobility ?

Ans. When an electric field E is applied to a semiconductor, the rate at which a current carrier gains momentum from the field = eE. The rate at which the carrier loses momentum through scattering = $\frac{m_{eff}\ v}{\tau}$ where m_{eff} is the effective mass of the carrier and τ is momentum relaxation time. In the steady state the rate of gain of momentum from the electric field is equal to the rate of loss of momentum through scattering

i.e. $$eE = \frac{m_{eff}\ v}{\tau}$$

where v is the drift velocity of electrons

or $$\frac{v}{E} = \frac{e\tau}{m_{eff}}$$

or $$\mu = \frac{e\tau}{m_{eff}}$$

Here μ is the mobility of carrier which is defined as the drift velocity per unit electric field intensity.

CHAPTER AT A GLANCE

1. Bloch Function is solution of Schrodinger wave equation for the undefined periodic potential in the potential well.

2. Kronig and Penny model's basic assumption is that the potential energy of the electron in the metals is a periodic array of square well with periodicity same as that of lattice.

3. The Band Structure of sold crystal is due to motion of electron in the periodic potential due to con core of the crystal.

4. The Effective mass of election is given by

$$m_{eff} = -\left(\frac{\hbar^2}{\frac{d^2E}{dk^2}}\right)$$

This mass is positive near the bottom of band, where the currature is positive. But near the top where the band curvature is negative, the effective mass is negative. The effective mass is different from the free mass because of the effect of the lattice force on the electron.

5. A Hole exists in a band which is completely full, with one vacant state. The hole acts as a particle of positive charge *i.e.*

6. Fermi level is the term used to describe the top of the collection of electron energy levels at zero Kelvin.

7. Valence band is the highest range of electronic energies in which electrons are normally opresent at zero Kelvin while the conduction band is the lowest range of vacant electronic states.

8. Kroning – Penny model tells us about the discountinuities in energy when the wave number $\bar{k}$ satisfies the condition

$$\bar{k} = n\frac{\Pi}{a} \text{ where } n = \pm 1, \pm 2, \pm 3, \ldots\ldots$$

9. $\bar{E}$ Versus $\bar{k}$ graph shows that an electron has allowed energy values in the region has allowed energy values in the region between $\frac{-\Pi}{a}$ to $+\frac{-\Pi}{a}$. This region is known as first Brillowin zone.

10. The second Brillown Zone for a two dimensionale lattice is represented by $k_x = \pm\frac{2\Pi}{a}$ and $k_y = \pm\frac{2\Pi}{a}$ excluding the space occupied by the first Brillowing zone.

11. The energies gap or forbidden band represents energies which the electrons cannot occupy.

12. Inrinsic semiconductors are those semiconductors in which the shifting of electons from valence band to conduction band and the production of holes in the valence band are achieved purely by thermal excitations.

13. Extrinsic Semiconductors are those semiconductors in which the conductivity is increased by adding pentavalent or trivalent atoms introduced by donar and acceptor impurities with locked energy levels near top or bottom of the for bidden gap.

14. N- type semiunductor is one in which the current conduction is due to excess of electrons whereas in **P-type semianductor,** conduction is by holes.

15. Mobility of charge carriers is defined as the drift velocity of a charge carrier produced due to unit of electric field strength.

16. Hall Effect is the production of a potential difference across a conductor or a semiconductor, transverse to an electric current in the conductor and to an applied magnetic field perpendicular to the current.

17. Hall Coefficient is defined as the ratio of the induced electric field to the product of the current density and applied magnetic field.

MULTIPLE CHOICE QUESTIONS

Choose the correct alternative for each question given below :

1. The conductivity of a semiconductor increases with increase in temperature because :

(a) number density of free current carriers increases

(b) relaxation time increases

(c) both number density of carriers and relaxation time increases

(d) number density of current carriers increases relaxation time decreases but effect of decrease in relaxation time is much less than increase in number density

2. **In band theory of solids :**

(a) the potential is taken constant inside the metal

(b) the potential is variable inside the metal

(c) the potential is taken infinite inside the metal

(d) potential is taken periodic inside the metal

3. **The effective mass of electron is :**

(a) $\dfrac{\hbar^2}{\left(\dfrac{dE}{dk}\right)}$ (b) $\dfrac{\hbar^2}{\left(\dfrac{d^2E}{dk^2}\right)}$

(c) $\dfrac{h}{\left(\dfrac{d^2E}{dk^2}\right)}$ (d) $\dfrac{h}{\left(\dfrac{dE}{dk}\right)}$

4. **The effective mass of electron is :**

(a) equal to actual mass of electron

(b) less than actual mass of electron

(c) greater than the actual mass of electron

(d) sometimes actual, sometimes less and sometimes equal to actual mass of the electron

5. **In Kronig-Penny model, if P << 1 the energy of the lowest energy band is**

(a) $E = \dfrac{\hbar^2 mP}{a^2}$ (b) $E = \dfrac{\hbar^2 P}{ma^2}$

(c) $E = \dfrac{a^2 \hbar P}{m}$ (d) $E = \dfrac{ma^2 P}{\hbar}$

6. **If σ_1 and σ_2 are the conductivities due to electron and holes and R_e and R_H the Hall constants then resulting expression is :**

(a) $R = \dfrac{R_e\,\sigma_e + R_h\,\sigma_h}{\sigma_e + \sigma_h}$ (b) $R = \dfrac{R_e\,\sigma_e^2 + R_h\,\sigma_h^2}{(\sigma_e + \sigma_h)^2}$

(c) $R = \dfrac{R_e\,\sigma_e + R_h\,\sigma_e}{(\sigma_h + \sigma_e)}$ (d) $R = \dfrac{R_e\,\sigma_h^2 + R_h\,\sigma_e^2}{(\sigma_e - \sigma_h)^2}$

7. **The conduction band is :**

(a) forbidden energy gap

(b) valence band

(c) a range of energies corresponding to the energies of the free electrons

(d) not an allowed energy band

8. In Kronig-Penny model, in one dimensional lattice the energy discontinuities occur when :

(a) $k = \pm n \frac{\pi}{a}$ (b) $k = \pm n\pi$

(c) $k = \pm \frac{n\pi}{2a}$ (d) $k = \pm \frac{3n\pi}{2a}$

9. In Kronig-Penny model as P increases

(a) width of allowed band decreases

(b) width of allowed band increases

(c) width of allowed band remains unchanged

(d) none.

10. At room temperature the conductivity of a semiconductor in Siemens per metre lies in the range of

(a) 100 to 10 (b) 1000 to 1

(c) 10^3 to 10^{-4} (d) 10^8 to 10^5

11. The Fermi level for an intrinsic semiconductor at T = 0K is :

(a) near the middle of the band gap

(b) far below the middle of band gap

(c) far above the middle of the band gap

(d) none of the above.

12. Donar type impurity is formed by adding impurity of valency :

(a) 3 (b) 4

(c) 5 (d) 6

13. Kronig-Penny model of solids is :

(a) parabolic type interactions potential for valence electron

(b) an improvement upon the free electron model

(c) only of academic interest as it solves no problem

(d) square well type periodic potential for valence electron

14. A pure semiconductor behaves as an insulator at

(a) room temperature (b) Boyle's temperature

(c) is independent of temperature (d) 0*K*

15. Measurement of Hall Coefficient enables the determination of

(a) mobility of charge carriers (b) Type of conductivity and concentration

(c) Temperature Coefficient and (d) None of above

(e) Thermal conductivity

16. **Hall Effect may be used for which of the following**
    (a) Determining the carrier concentration
    (b) Determining whether the semiconducter is n-type or p-type
    (c) Calculating the mobility
    (d) All of the above.

17. **Hall voltage is directly proportional to**
    (a) Current (b) Electric field
    (c) Magnetic flux density (d) All of the above

18. **Hall probe is mode up of**
    (a) metals (b) non metals
    (c) radoactive substance (d) semiconductor

19. **Measurement of Hall coefficient in a semiconductor provides information on the**
    (a) Sign and mass of charge carriers
    (b) Mass and concentration of charge carriers
    (c) Sign of charge carriers
    (d) Sign and concentration of charge carriers

20. **The Hall coefficient of intrinsic semiconductor is**
    (a) Positive under all conditions (b) Negative under all conditions
    (c) Zero under all conditions (d) non of the above

21. **The majority carriers is an n – Type Semiconductor have an average drift velocity in Hall effect acts in the direction**
    (a) $\vec{V} \times \vec{B}$ (b) $\vec{B} \times \vec{V}$
    (c) along $\vec{V}$ (d) Opposite to $\vec{V}$

Answers

1.	(d)	2.	(a)	3.	(b)	4.	(d)	5.	(b)
6.	(b)	7.	(c)	8.	(a)	9.	(a)	10	(c)
11.	(a)	12.	(c)	13.	(d)	14.	(d)	15.	(b)
16.	(b)	17.	(c)	18.	(d)	19.	(d)	20.	(b)

SHORT ANSWER QUESTIONS

1. What is the basis of band theory of solid ?
2. Give a typical value of band gap energies for a solid.
3. Effective mass of the electron may be negative. Is it true ?
4. Draw the infinite periodic one demensunal square well potential as predicted by Kronig and Penny.
5. Why is Kronig – Penny model useful ?

6. What are semiconductors. Give examples
7. What are elemental and compound semiconductors Also give their examples.
8. Give the position of Fermi level in an intrinsic semiconductor at zero Kelvin.
9. What is an extrinsic semiconductor ?
10. What do you mean by donars and acceptors ?
11. How is Hall coefficient related with carrier concentration ?
12. On what factors does the Hall coefficient's sign depend ?
13. Is it possible to measure Hall coefficient for metals?
14. In what units is Hall coefficient measured ?
15. How does mobility depend on electrical conductivity ?
16. Why is Four probe method preferred over other conventional methods for measuring resistivity ?
17. What happens to Hall coefficient when number of charge carriers is decreased?

LONG ANSWER QUESTIONS

1. Discuss the periodicity character of potential in a crystal. State Bloch theorem in this reference.
2. Discuss Kroning-Penny model. Using this model show that the energy spectrum of electron consists of a number of allowed energy bands separated by forbidden regions
3. (a) Distinguish between metals, insulators and semiconductors. Why a semiconductor acts as an insulator at zero Kelvin ?

   (b) While the conductivity of a metal decreases with rise of temperature but the conductivity of a semiconductor increases with rise of temperature. Explain ?
4. Starting with the solution of Schrodinger's equation for one dimensional periodic lattice

$$\frac{P\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

where $\alpha = \sqrt{\frac{2mE}{\hbar^2}}$, discuss the formation of energy boundaries solids.

Also draw the energy versus wave vector graph to highlight the main the conclusions of Kronig – Penny's model.

5. (a) What are the conclusions of Kronig –Penny model for energy band structure of solids ?

   (b) What is the effect of changing the binding energy of an electron on the energy bonds ?

6. What are valence and conduction band ? Explain why a solid whose energy bands are full cannot be a metal ?

7. What are Brillouin Zones d/p? Show that the existence of energy groups at the boundaries of the Brillouin Zone one dimensional lattice is equivalent to the condition of Bragg's reflection of electron waves Discuss the importance of first Brillouin zone.

8. What are intrinsic and extrinsic semiconductors ? Discuss the locations of Fermi levels under suitable limiting conditions and give the necessary theory.

9. Derive the expression for velocity of electron and draw a graph between velocity and wave vector.

10. What do you mean by effective mass? Deduce the relation for effective mass of an electron. Show how it is different from rest mass of the electron.

11. Differentiate n–type and p–type semiconductors. How does the conductivity and mobility of electrons and holes change with temperature ?

12. Obtain an expression for density of electrons in conduction bond of n–type semiconductor.

13. Obtain an expression for density of holes in conduction band of p-type semiconductor.

14. Discuss the motion of an electron in one dimension according to band theory and show how the energy, velocity and effective mass vary as function of wave vector.

15. Explain Hall effect ? Derive an expression in for the Hall coefficient of semiconductor on two band model of carriers. Discuss Four probe method and uses of Hall Effect.

UNSOLVED NUMERICAL PROBLEMS

1. An insulator has an optical absorption which occurs for all wavelengths shorter than 1800 Å. Find the width of the forbidden energy band for the insulator.

[Ans. 6.9 eV]

2. Determine the concentration of conduction electrons per m^3 in pure silicon, if its conductivity is $5 \times 10^5\ \Omega^{-1}\ m^{-1}$. Electron and hole mobilities are 0.16 and 0.08 m^2/Vs respectively. [Ans. 1.31×10^{25}]

3. The Fermi level in potassium is 2.1 eV at a particular temperature. Calculate the number of free electrons per unit volume in potassium at the same temperature. Given $a = \frac{\pi}{3}$. [Ans. 1.31×10^{28} electrons/m^3]

4. Calculate the concentration of electrons and holes in an n-type semiconductor, if the donar density is 10^{20} atoms/m^3 and the intrinsic carrier concentration is $2.5 \times 10^{19}/m^3$ at room temperature. [Ans. 6.25×10^{18} atoms m^{-3}]

[Hints : $I_c = 2\pi r\ H_c = 2 \times 3.14 \times 0.3 \times 10^{-3} \times 7 \times 10^3 = 13.19\ A$]

5. The energy near the valence band edge of the crystal is given by $E = -Ak^2$ where $A = 10^{-39}\ J\ m^2$. Find the effective mass of the electron with wave vector having magnitude of $10^{10}\ m^{-1}$. [Ans. $-0.55 \times 10^{-29}\ kg$]

6. In an n-type semiconductor, the Fermi level lies 0.4 eV below the conduction band. If the concentration of donar atoms is doubled, find the new position of Fermi level. [Ans. 0.379 eV]

7. A copper strip 4.0 cm wide and 0.5 mm thick is placed in a magnetic field of induction 2.0 Tesla. If a current of 100 A is set up in the strip, how much Hall potential difference appears across the strip ? One cubic metre of copper strip contains 8.4×10^{28} electrons. [Ans. 29.7×10^{-6} V]

8. A semi-conducting crystal 12 mm long, 5 mm wide and 1 mm thick has a magnetic induction of 0.5 Tesla, applied from front to back perpendicular to the largest face. When a current of 20 mA flows lengthwise through the specimen, the voltage measured across its width is found to be 37 μV. What is the Hall coefficient of the semiconductor ? Estimate what the voltage would have been if a specimen of copper of smaller dimensions and with the same 20 mA current flowing along its length is placed in the same magnetic field. The number of atoms per unit volume is given to be $8.5 \times 10^{28}\ m^{-3}$. [Ans. $R_H = 3.7 \times 10^{-6}\ C^{-1}\ m^3$ and $V_H = 0.74 \times 10^{-9}$ V]

□□□

Chapter 7

SUPER CONDUCTIVITY

7.1 INTRODUCTION

We know that conductors (metals) offer resistance to the flow of current through them and resistance of conductors decreases with increase of temperature. The electrical resistance of some elements, alloys or chemical compounds drops suddenly to zero when their specimens are cooled to a sufficiently low temperature (*i.e.* temperature in the liquid helium range) and current flow without power loss and decay with time period of 10^4 to 10^5 years. This phenomenon was first discovered by Kammerlingh Onnes in 1911. He observed that resistance of pure mercury drops to zero at temperature 4.2 K. As this transition occurs over a small temperature range of about 0.05°C, the phenomenon is given the name **superconductivity.** The substances showing this property are called superconductors as shown in Fig. (7.1).

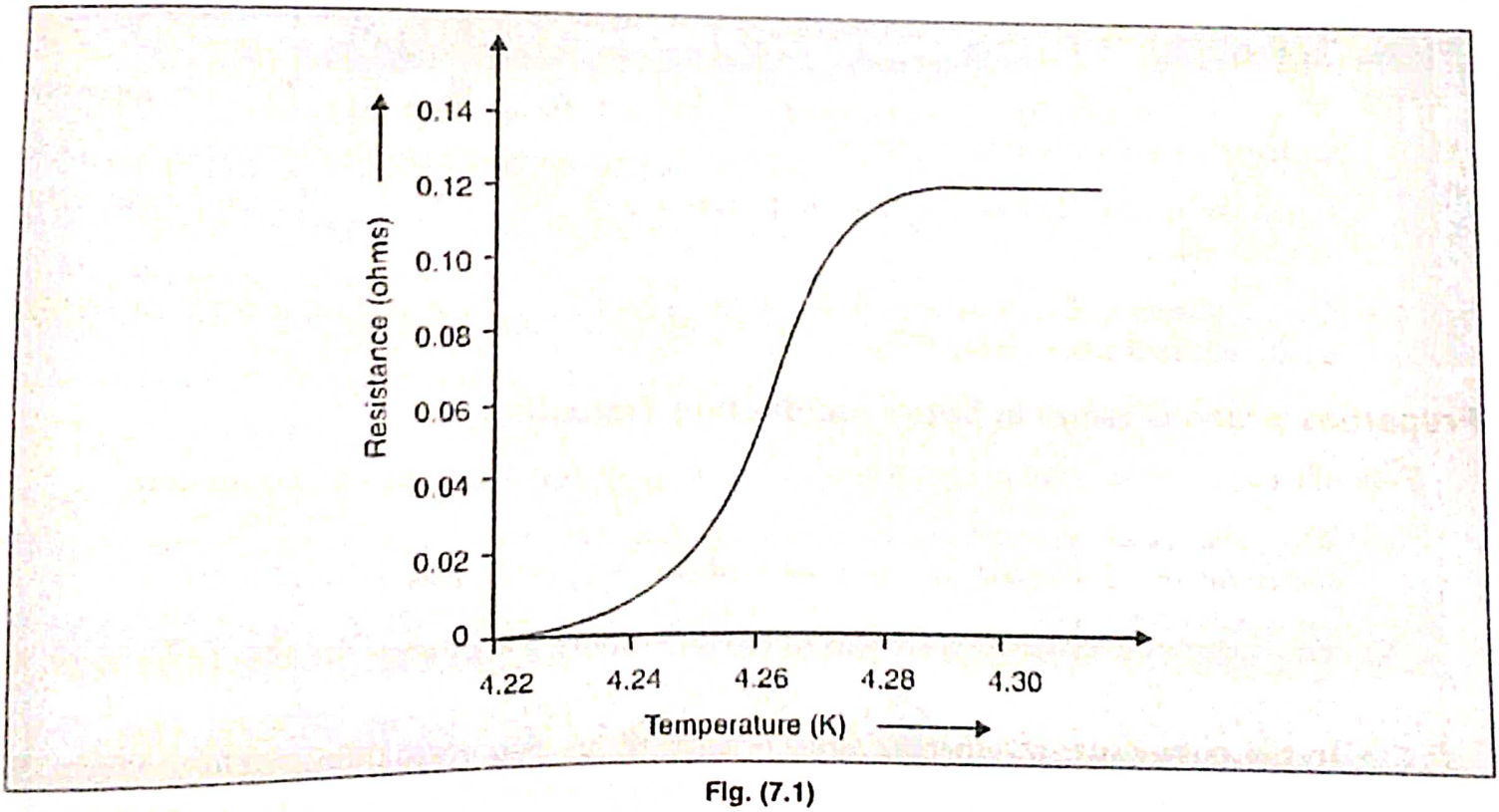


Fig. (7.1)

Thus superconductivity is defined as the phenomenon, in which the electrical resistance of a substance drops suddenly to zero when it is cooled below a certain temperature (T_c).

The temperature at which the normal metal passes into super conducting state is called the **transition temperature** or **critical temperature** (T_c).

There are at least 25 super conducting elements and a much larger number of super conducting compounds and alloys.

The metals (i.e. Silver, Gold and Copper) which at normal temperature are the best conductors, are not superconductors.

7.2 EXPERIMENTAL RESULTS

After the discovery of superconductivity, a large number of experiments were performed to find out, the dependence on external conditions like current, magnetic field, nature of substance, presence of impurity etc. The observations made from these experiments are given below.

Properties which do not Change in Super conducting Transitions

Following are the various properties which do not change in superconductivity transitions :

(i) The X-ray diffraction pattern is same both above and below the critical temperature which shows that during super conducting transition, the crystal structure of the material remains same.

(ii) The change in intensity of diffracted X-rays was not noticeable, which indicates that during super conducting transition, the electronic structure remains almost the same.

(iii) There is no appreciable change in the reflectivity either in visible or in infrared region.

(iv) There is no change in absorption of fast or slow electrons. The photoelectric properties are also unchanged.

(v) The elastic and thermal expansion properties do not change with super conducting transition.

(vi) In the absence of a magnetic field, there is no latent heat and no change in volume at super conducting transition.

Properties which Change in Super conducting Transition

Following are the various properties which change in super conducting transition.

(i) The electrical properties of material get totally changed *i.e.* above critical temperature (T_c), resistance is more and below T_c resistance is zero.

(ii) The magnetic properties of the material undergo a change in the same way as electric properties.

In the pure super-conducting state practically no magnetic flux is able to enter the metals which thus behaves as if it had zero permeability or strong diamagnetic susceptibility. When super-conductivity is destroyed a magnetic field, the magnetic behavior becomes complicated.

(iii) The specific heat changes discontinuously at the transition temperature. There is small change of volume at the transition in the presence of magnetic field.

(iv) All thermoelectric effects (Seebeck, Peltier, Thomson) disappear in superconductivity state.

(v) The thermal conductivity changes discontinuously when the superconductivity is destroyed in magnetic field. It is lower in the super conducting state for pure metals put higher for certain alloys.

7.3 CRITICAL TEMPERATURE

The temperature at which the normal metal passes into superconducting state is called the transition temperature or critical temperature (T_c).

There are atleast 25 superconducting elements and a much larger number of superconducting compounds and alloys. Some of them are given below along with their critical temperatures.

Superconductivity is absent in ferromagnetic metals, monovalent metals and rare earth elements excepts Lanthanum.

Table : Superconducting transition temperature for selected elements, compounds and alloys.

Element	$T_c(K)$	Elements	$T_c(K)$
Technetium	11.2	Nb_3Ge	23.2
Niobium	9.46	Nb_3Ga	20.3
Lead	7.18	Nb_3Sn	18.05
Tantalum	4.48	NbN	16.0
Mercury	4.15	MoN	12.0
Indium	3.41	MO_3Ir	8.8
Aluminium	1.19	$NiBi$	4.25
Cadmium	0.56	$AuBe$	2.64
Titanium	0.40	Ti_2C_o	3.44
Iridium	0.14	TiC_o	0.71
Tungsten	0.01	$BaBi_3$	5.59
Tin	3.73	$YBa_2Cu_3O_7$	90
Thallium	2.38	$NbTi$	10
Thorium	1.39	$Nb_3Al_{0.8}Ge_{0.2}$	20.05
Zinc	0.91	Nb_3Al	17.5
Uranium	0.8	V_3Si	17.1

Some of the observations about the material to show superconductivity are given below.

The variation of resistivity of metals with temperature is shown in Fig. (7.2).

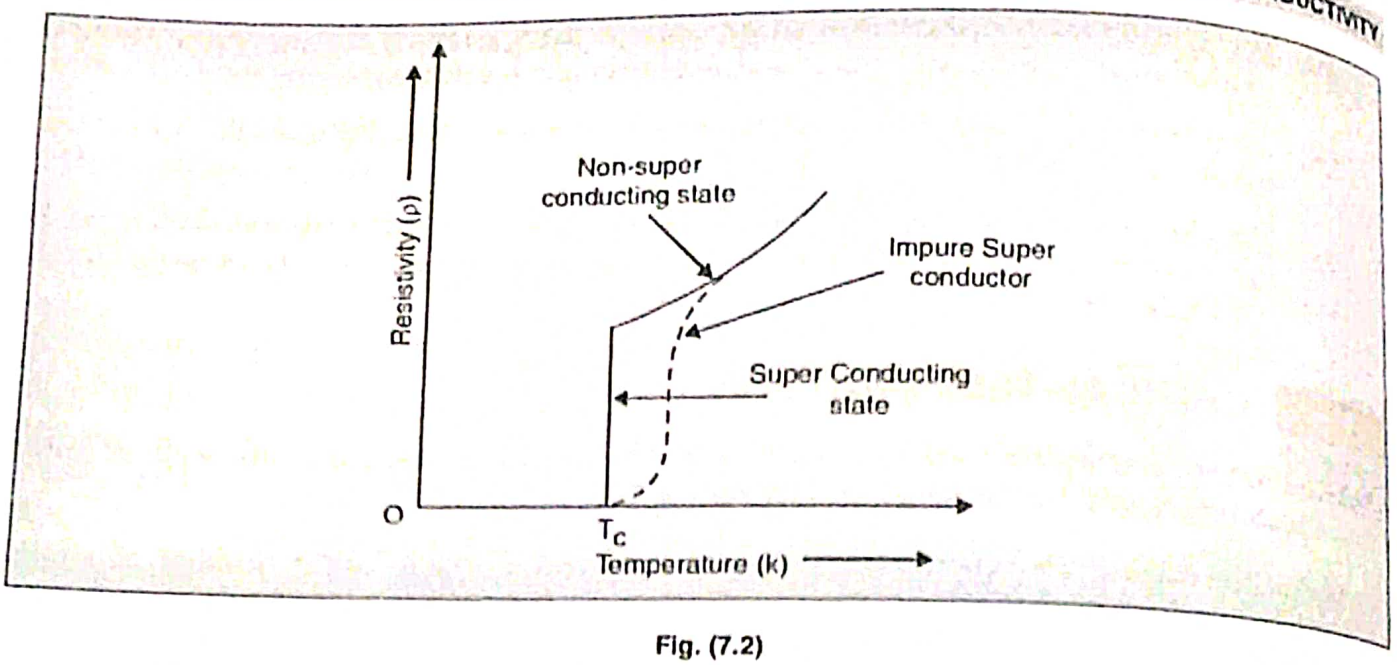


Fig. (7.2)

The variation of critical temperature (T_c) with number of valence electrons (Z) of metallic substances is shown in Fig. (7.3).

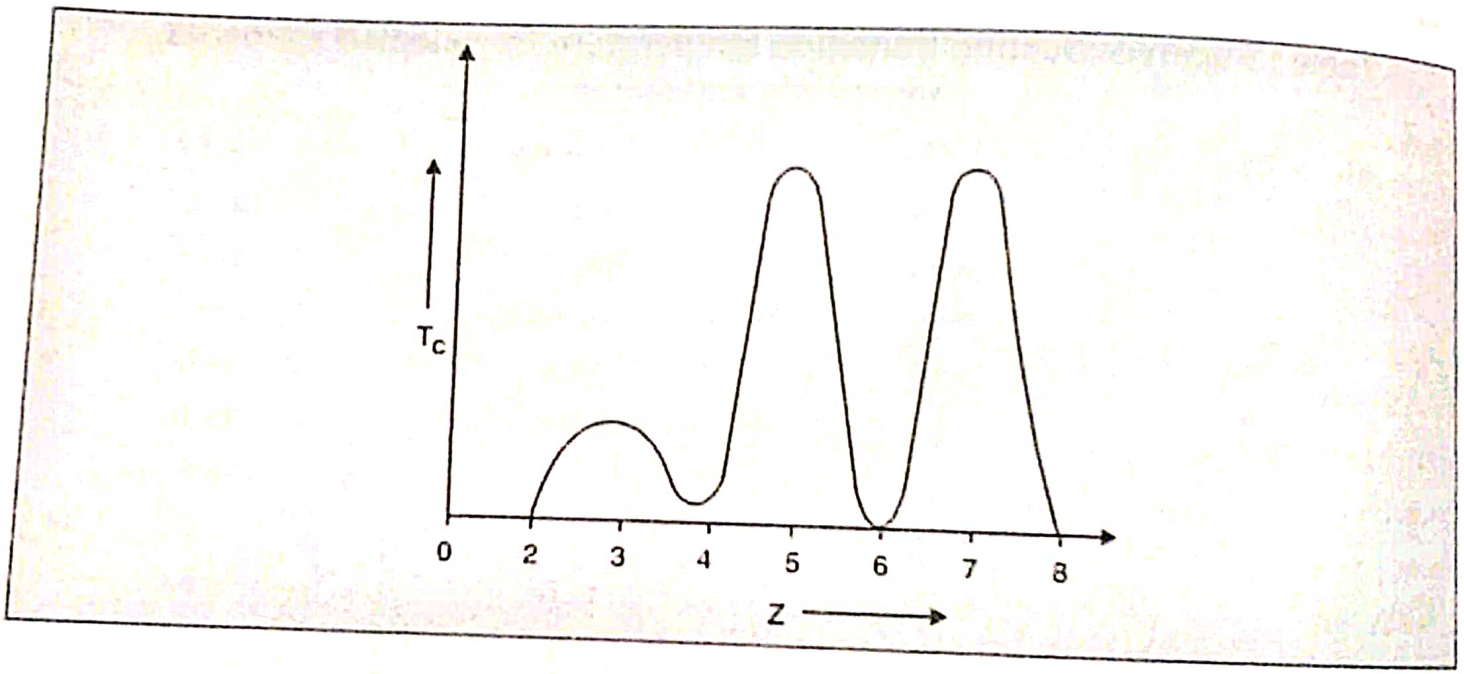


Fig. (7.3)

Following information is drawn from these graphs shown in Figs (7.2 & 7.3), table and other experimental observations.

(i) In an ordinary metal, there exists a small resistivity (residual) even at lower temperature. The residual resistivity depends on impurities present in the metal. The more impure is metal, the more is residual resistivity.

(ii) The critical temperature is the characteristic of a super conducting material. This is different for different superconducting materials.

(iii) If the temperature of a superconducting material is increased. The material transforms into a normal material above the critical temperature.

(iv) The materials (metallic substances) whose number of valence electrons Z lies between 2 to 8 generally show superconductivity.

(v) Critical temperature T_c of the superconducting materials shows maximum values for $Z = 3$, 5 and 7 as shown in Fig. (7.3).

(vi) The graph between critical temperature T_c and Z^2 is a straight line.

(vii) Critical temperature T_c varies inversely as the atomic mass of super conducting materials.

(viii) The material having high normal resistivities show the superconductivity.

7.4 CRITICAL MAGNETIC FIELD

In 1913, Kammerlingh Onnes observed that superconductivity vanishes if a sufficiently strong magnetic field is applied. **The minimum applied magnetic field necessary to destroy superconductivity and restore the normal resistivity is called critical magnetic field (H_c).** When the applied magnetic field exceeds the critical value H_c, the superconducting state is destroyed and the material goes into normal state. The critical magnetic field (H_c) depends on temperature. The variation of critical magnetic field with temperature is shown in Fig. (7.4). This type of graph is known as magnetic phase diagram. A specimen is super conducting below the curve and in normal conducting state above the curve. As observed from (Fig. 7.4) that normal conducting state of the material is restored if the magnetic field is greater than the critical value (H_o) or temperature of the specimen is raised above critical temperature T_c. In other words, for the super conducting state to exist, there must be a suitable combination of temperature and magnetic field. For a given substance, the value of H_C decreases as temperature increases from $T = 0K$ to T_c (critical temperature).

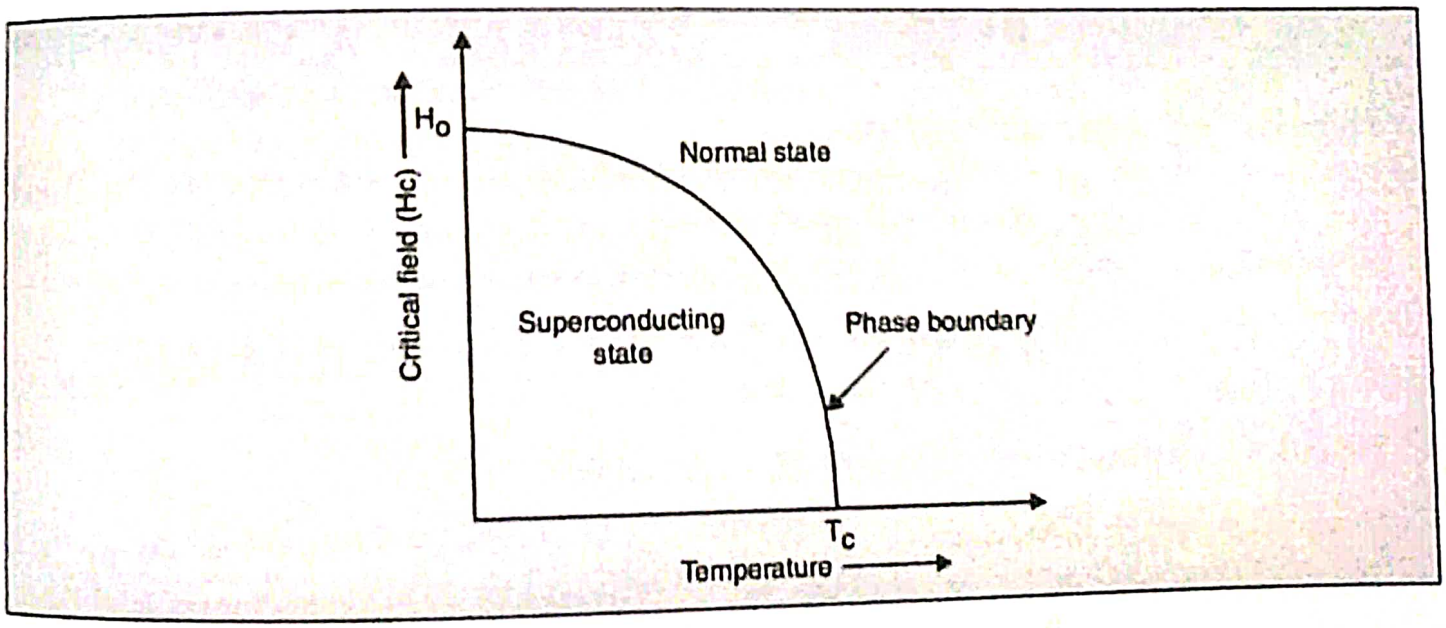


Fig. (7.4)

The curve is nearly parabolic and can be represented as

$$H_c = H_o\left(1 - \frac{T^2}{Tc^2}\right) \qquad \ldots(7.1)$$

where H_0 is critical field at $0K$, H_c is critical field at temperature T and T_c is critical temperature.

According to this equation (7.1)

(*i*) At $T = 0K$

$$H_c = H_0 = \left(1 - \frac{0}{T^2}\right) = H_0(1 - 0) = H_0$$

(*ii*) At $T = T_c$

$$H_c = H_0 \left(1 - \frac{T_c^2}{T_c^2}\right) = H_0(1 - 1) = H_0(0) = 0$$

In general, higher is the value of T_c. The higher is the value of H_c.

Silsbee Effect

We know that when current is passed through a conductor it produces magnetic field. If the magnetic field produced due to current is more than critical magnetic field H_c, the super conducting state of the material may be destroyed even though there is no external magnetic field around superconductor. This limits the maximum amount of current that can be passed through a superconductor. This maximum allowable current is called critical current I_c.

Let current (I) is passed through a super conducting wire of radius (r), then magnetic flux density at the surface of wire is given as

$$B = \frac{\mu_0 I}{2\pi r} \qquad \ldots(7.2)$$

Magnetic field at the surface of wire

$$H = \frac{B}{\mu_0}$$

$$H = \left(\frac{\mu_0 I}{2\pi r}\right) \frac{1}{\mu_0} = \frac{I}{2\pi r} \qquad \ldots(7.3) \text{ [Using eqn. (7.2)]}$$

When $I = I_c$ = critical current then $H = H_c$ = critical field.

Thus above eqn. (7.3), becomes

$$H_c = \frac{I_c}{2\pi r} \qquad \ldots(7.4)$$

This equation is called Silsbee Rule. Silsbee suggested that the important factor in causing destruction of superconductivity was the magnetic field associated with the current, rather than the value of current itself. The destruction of superconductivity is actually field controlled effect.

7.5 MEISSNER EFFECT

In 1993, Meissner and Ochsenfeld found that if a superconductor is cooled in a magnetic field, below critical temperature (transition temperature) corresponding to that field, then the lines of magnetic induction are expelled from the material, at the transition as shown in Fig. (7.5*b*). This effect is called Meissner effect.

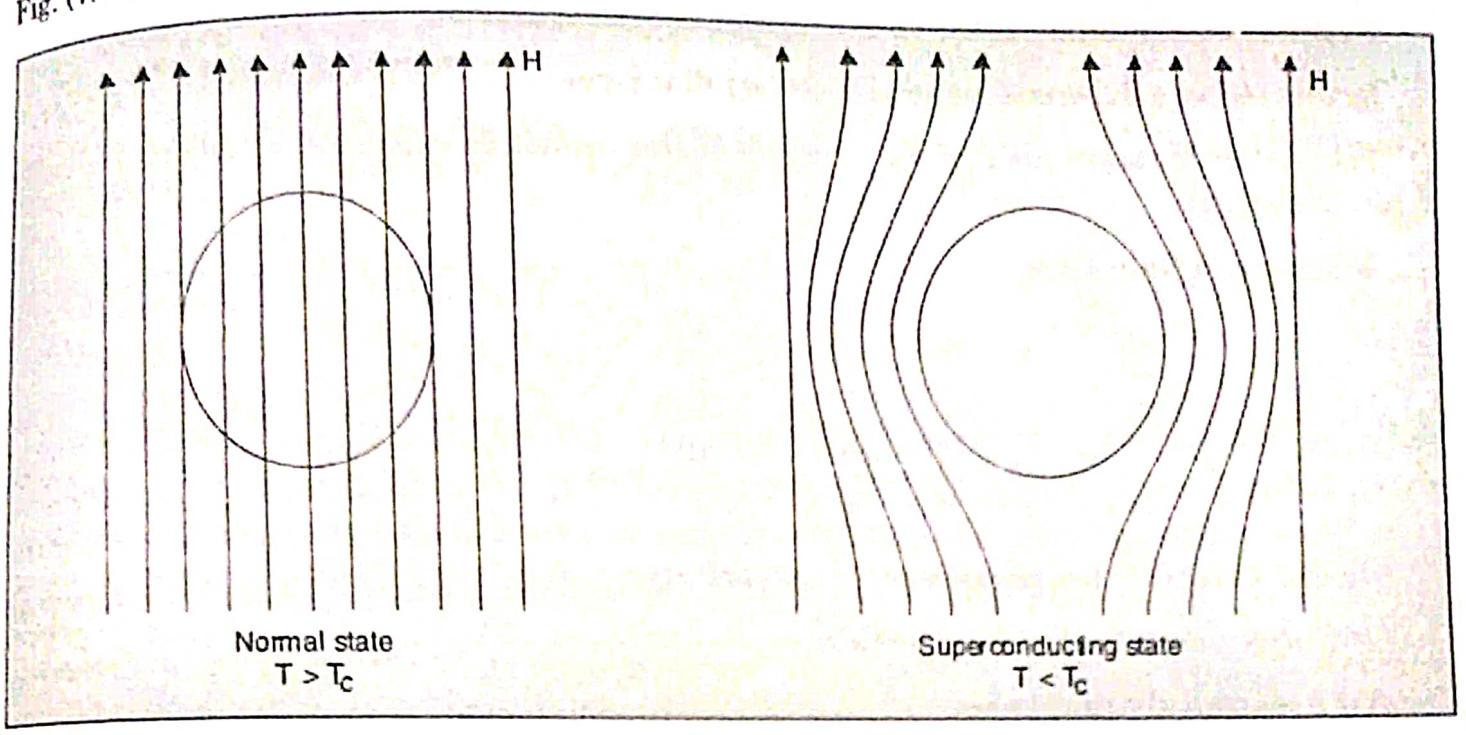


Fig. (7.5a) Fig. (7.5b)

Thus expulsion of magnetic lines of force from a superconducting material when it is cooled below transition temperature in a magnetic field is called Meissner effect.

Fig. (7.5*a*) shows superconductor in normal state and magnetic lines of force pass through it. Fig. (7.5*b*) shows superconducting state in which magnetic lines of force are expelled out of specimen. Meissner effect is reversible, when the temperature is raised from below critical temperature (T_c) then magnetic flux suddenly penetrates the specimen. Since the magnetic induction in a superconductor is zero, hence a superconductor is a **perfect diamagnetic.**

We know that magnetic flux density inside the conductor placed in a magnetic field is given as

$$B = \mu_0(H + I) \qquad \ldots(7.5)$$

where H is magnetising field intensity and I is intensity of magnetisation.

For a superconductor, $B = 0$

$\therefore$ Eqn. (7.5) becomes

$$\mu(H + I) = 0$$

or $$H + I = 0$$

or $$I = -H \qquad \ldots(7.6)$$

Magnetic susceptibility (χ_m)

$$\chi_m = \frac{I}{H} = \frac{-H}{H} = -1 \qquad \text{Using eqn. (7.6)}$$

$$\therefore \quad \chi_m = -1 \qquad \ldots(7.7)$$

Negative susceptibility is the characteristic of diamagnetism.

In this sense, a superconductor is a perfect diamagnet.

The perfect diamagnetism of the superconductor cannot be explained simply on the basis of zero resistivity.

According to Ohm's law

$$V = IR \quad \text{and} \quad E = \frac{V}{d}$$

$$\therefore \quad E = \frac{IR}{d} = \frac{JAR}{d} = J\left(\frac{AR}{d}\right) = \rho J$$

where I = current, R = Resistance, ρ = resistivity,

J = Current density, E = Electric field

A = Area and d = thickness.

$$\therefore \quad E = \rho J \qquad \ldots(7.8)$$

For finite J and $\rho = 0$, E should be zero.

If $E = 0$ also, then Maxwell's equation

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \text{ becomes}$$

$$\frac{\partial \vec{B}}{\partial t} = 0$$

or $\qquad B = \text{constant.}$

It means, the magnetic flux through a perfect conductor does not change even if it is cooled to its critical temperature. This is in contradiction to Meissner effect.

Hence state of zero resistivity and perfect diamagnetism are mutually independent of each other.

Thus for a superconductor

$$E = 0 \text{ (Absence of resistivity)}$$

and $\qquad B = 0$ Meissner effect

Hence superconductivity is not only a strong diamagnetism, but a new type of dimagnetism.

7.6 TYPE-I AND TYPE-II SUPERCONDUCTORS

Superconductors are classified into two types, based on their magnetic behaviour. These two types are :

(i) Type-I superconductors (or soft superconductors)

(ii) Type-II superconductors (or hard superconductors)

(I) Type-I Superconductors :

Type-I superconductors are also known as soft superconductors. The dependence of magnetization of a superconductor of type-I as a function of external field H is shown in (Fig. 7.6).

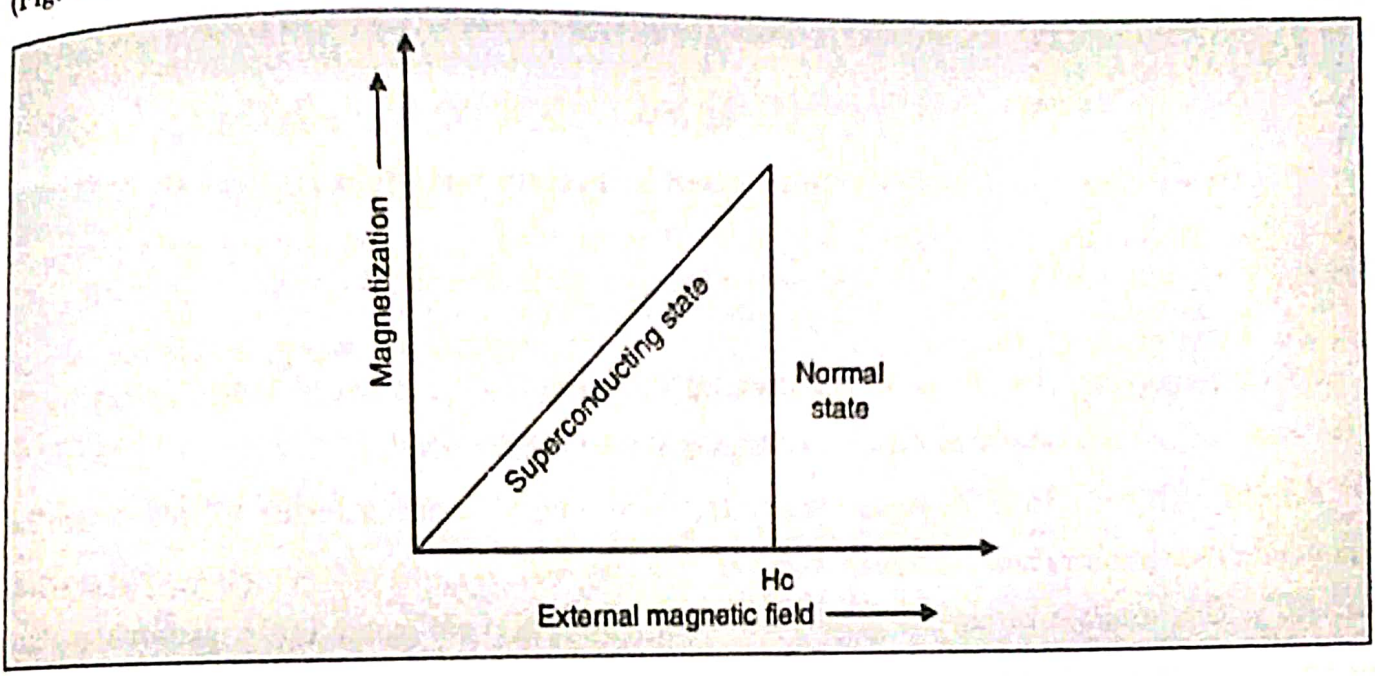


Fig. (7.6)

They are perfectly diamagnetic and follow Meissner's effect very strictly and transition from superconducting to normal state is abrupt. They completely expel the magnetic field from interior of the superconducting phase upto critical field strength H_c. The magnetization of superconductor grows in proportion to the external magnetic field H and then abruptly drops to zero as soon as the applied field H exceeds H_c.

If external applied field $H < H_c$, type-I superconductors are in superconducting state and perfect diamagnet. But as soon as H exceeds H_c, the superconductor enters in normal state and its diamagnetic property disappears and the magnetic flux penetrates through the superconductor. The value of H_c for most of type-I superconductors is very low (about 0.1 tesla). Aluminium, lead and indium are examples of type-I superconductors. Type-I superconductors have limited applications in technology because of their lower value of H_c.

(II) Type-II Superconductors

Type-II superconductors are also known as hard superconductors and are quite different from type-I superconductors. The magnetization curve of type-II superconductor is shown in Fig. (7.7).

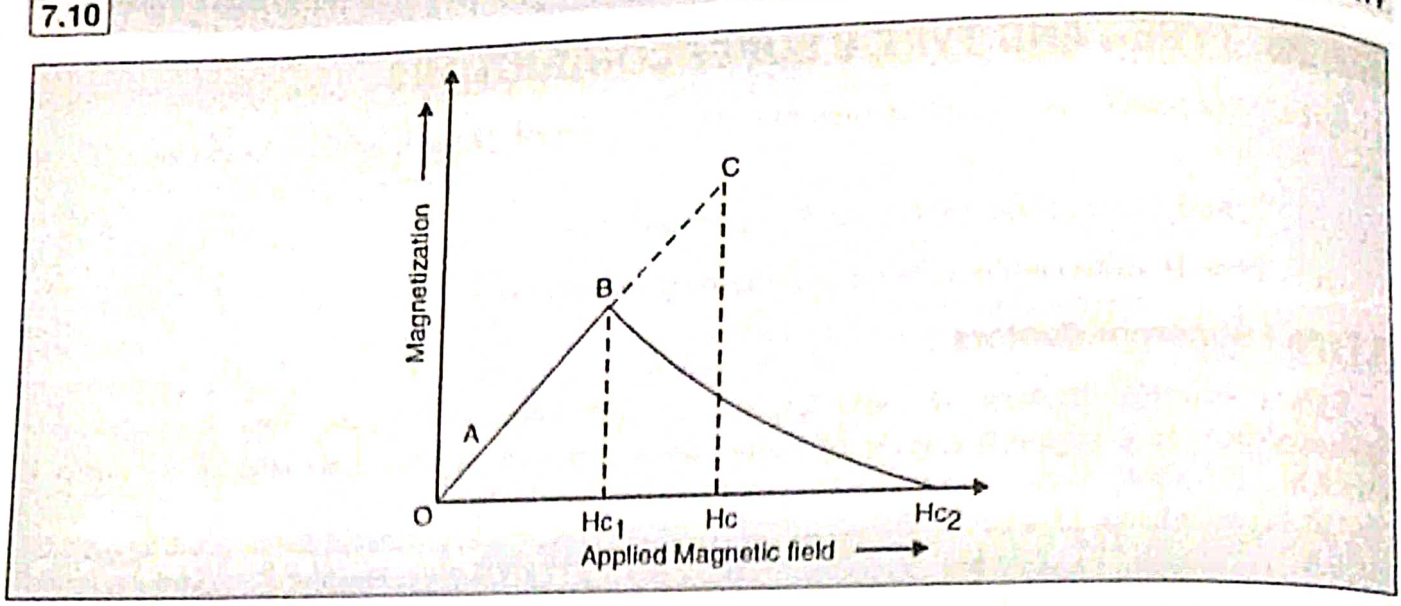


Fig. (7.7)

The type-II superconductor is characterised by two critical fields H_{c_1} and H_{c_2}. They do not follow Meissner effect strictly. Also type-II superconductors do not abruptly jumps to normal state as type-I superconductor as field is increased. For values of field below H_{c_1}, the superconductors expels the magnetic field from its body (material) completely and behaves as a perfect diamagnet. The curve is represented by AB and H_{c_1} is called lower critical field. The material is thus totally in super conducting state in this region.

As the magnetic field increases from H_{c_1}, the magnetic lines begin to penetrate the material. This penetration increases until H_{c_2} is reached. H_{c_2} is called upper critical field. At H_{c_2}, the magnetization becomes zero and external field completely penetrates the superconductor and destroy the superconductivity.

Between two critical fields H_{c_1} and H_{c_2} the field inside the specimen is not zero and hence Meissner effect is not obeyed completely. Since a large magnetic field is required to destroy the super-conducting properties of the specimen hence these superconductors are called hard superconductors.

The specimen is said to be in the vertex region or mixed state between H_{c_1} and H_{c_2}. In this region specimen is a mixture of super-conducting and non super-conducting regions.

After H_{c_2} the material turns to normal state. Type-II superconductors have many practical applications like (*i*) They are used to make high field magnets for particle accelerators, fusion reactors etc.

Differences between Type-I and Type-II Superconductors

Type-I Superconductors	Type-II Superconductors
1. They are called soft superconductors.	1. They are called hard superconductors.
2. They strictly follow the Meissner effect.	2. They do not follow Meissner effect strictly.

3. Below critical field H_c, they exhibit perfect diamagnetism. As the magnetic field is increased beyond H_c, the field penetrates the material completely and the specimen is changed to normal state.	3. They exhibit perfect diamagnetism upto magnetic field H_{c_1} called lower critical magnetic field. Between H_{c_1} and H_{c_2} the specimen is in mixed state. Above H_{c_2} the specimen is normal conductor.
4. They abruptly jump to normal state once the magnetic field is increased higher than H_c.	4. They do not abruptly jump to normal state as magnetic field is increased.
5. The value H_c is very low, hence they have very limited applications in technology.	5. Because of relatively large field is required to destroy the superconductory, they have many practical applications.

7.7 LONDON'S EQUATION

To explain Meissner effect and zero resistivity F. London and H. London in 1934 proposed a macroscopic theory of superconductors. They derived two new field equations to explain Meissner effect and zero resistivity, which are known as London equations. The theory is based on the idea that a superconductor is composed of normal and super conducting electrons.

At superconducting temperature, the conduction is only due to superconducting electrons but as the temperature increases, the number of superconducting electrons decreases while the number of normal electrons increases.

Let m = mass of electron

$-e$ = charge on electron

n_s = number of super conducting electrons per unit volume

n_n = number of normal electrons per unit volume

v_s = drift velocity of superconducting electrons

$\vec{E}$ = Electric field.

According to Newton's second law, the equation of motion of electron inside a conductor is given as

$$\frac{md\vec{v}}{dt} = -e\vec{E} + \text{Resistive force} \qquad \ldots(7.9)$$

However for super conducting electrons there is no resistance. Hence resistive force is zero.

Therefore, eqn. (7.9) becomes

$$\frac{md\vec{v}_s}{dt} = -e\vec{E} \qquad \ldots(7.10)$$

The current density of super conducting electrons is given as

$$\vec{J}_s = -n_s e \vec{v}_s \qquad \ldots(7.11)$$

The negative sign shows that direction of current density is opposite to drift velocity of electrons.

From eqn. (7.11)

$$\frac{d\vec{J}_s}{dt} = -n_s e \frac{d\vec{v}_s}{dt}$$

or $$\frac{d\vec{J}_s}{dt} = -n_s e\left(-\frac{e\vec{E}}{m}\right) \qquad \text{using eqn. (7.10)}$$

or $$\frac{d\vec{J}_s}{dt} = \frac{n_s e^2}{m}\vec{E} \qquad \ldots(7.12)$$

This equation (7.12) is called **First London Equation.**

Taking curl of eqn. (7.12), we get

$$\frac{d}{dt}(\vec{\nabla} \times \vec{J}_s) = \frac{n_s e^2}{m}(\vec{\nabla} \times \vec{E}) \qquad \ldots(7.13)$$

From Maxwell equation, we can write

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{dt}$$

Putting this value in eqn. (7.13), we get

$$\frac{d}{dt}(\vec{\nabla} \times \vec{J}_s) = -\frac{n_s e^2}{m}\frac{\partial \vec{B}}{\partial t}$$

Integrating w.r.t. time, we get

$$\vec{\nabla} \times \vec{J}_s = -\frac{n_s e^2}{m}\vec{B} \qquad \ldots(7.14)$$

The magnetic flux density $\vec{B}$ is related to vector potential $\vec{A}$ as

$$\vec{B} = \vec{\nabla} \times \vec{A}$$

Putting this value in eqn. (7.14), we get

$$\vec{\nabla} \times \vec{J}_s = -\frac{n_s e^2}{m}(\vec{\nabla} \times \vec{A})$$

$$\vec{J}_s = \frac{-n_s e^2 \vec{A}}{m} \quad \text{...(7.15)}$$

or

This equation (7.15) is called **Second London Equation** and is only correct for superconductors.

We can explain both Meissner effect and flux penetration using London equations as follows :

The Ampere's Circuital Law in differential form

$$\vec{\nabla} \times \vec{B} = \mu_0 \vec{J}_s \quad \text{...(7.16)}$$

Taking curl both sides, wet get

$$\vec{\nabla} \times (\vec{\nabla} \times \vec{B}) = \mu_0 (\vec{\nabla} \times \vec{J}_s)$$

or $$\vec{\nabla}(\vec{\nabla} \cdot \vec{B}) - \nabla^2 \vec{B} = \mu_0 (\vec{\nabla} \times \vec{J}_s)$$

$$-\nabla^2 \vec{B} = \mu_0 (\vec{\nabla} \times \vec{J}_s) \qquad (\because \vec{\nabla} \cdot \vec{B} = 0)$$

or $$-\nabla^2 \vec{B} = -\mu_0 \left(\frac{n_s e^2}{m}\right) \vec{B}$$ Using eqn. (7.14)

or $$\nabla^2 \vec{B} = \left(\frac{\mu_0 n_s e^2}{m}\right) \vec{B}$$

or $$\nabla^2 \vec{B} = \frac{1}{\lambda^2} \vec{B} \quad \text{...(7.17)}$$

where $$\lambda = \sqrt{\frac{m}{\mu_0 n_s e^2}}$$

is called the London penetration depth. Its value ranges from 300 Å to 5000 Å. It is characteristic of the material.

Eqn. (7.17) in one dimension becomes

$$\frac{d^2 B}{dx^2} = \frac{1}{\lambda^2} B \quad \text{...(7.18)}$$

This is a simple differential equation which has solution

$$B = A_1 e^{-x/\lambda} + A_2 e^{x/\lambda}$$

where A_1 and A_2 are constants. These constants can be determined by applying boundary conditions.

The solution $A_{2e}^{x/\lambda}$ is discarded because it indicates that field increases as we move inside the superconductor. Therefore, the solution is

$$\therefore \quad B = B_{0e}^{-x/\lambda} \qquad \ldots(7.19)$$

where x is the distance from surface of the specimen and B_0 is magnetic flux density at the surface of superconductor. This equation shows that magnetic field inside the sample decreases exponentially with distance from the surface as shown in fig. (7.8).

For $x = \lambda$

Eqn. (7.19) becomes

$$B = B_0 e^{-1}$$

or
$$B = \frac{B_0}{e} \qquad \ldots(7.20)$$

Thus London penetration depth is defined as the measure of the distance from the surface of the superconductor at which the magnetic of decays to $\frac{1}{e}$ of its value at the surface of the superconductor.

If thickness x of the material is much less than the penetration depth

i.e. $x << \lambda$ or $\frac{x}{\lambda} \approx 0$

then e.g. (7.10) becomes

$$B \approx B_0$$

i.e. magnetic flux density everywhere inside the superconductor is constant and equal to the value at the surface of superconductor. This explains flux penetration.

If thickness x of the sample is much larger than penetration depth i.e. $x >> \lambda$ then

$$\frac{x}{\lambda} \approx \infty$$

or
$$e^{-x/\lambda} \approx e^{-\infty} = 0$$

$\therefore$ Eqn. (7.19) becomes

$$B \approx 0$$

Thus magnetic flux density inside the sample will zero *i.e.* Meissner Effect (Perfect diamagnetism) will be exhibited by the material.

Thus London equations explain flux penetration and Meissner effect successfully.

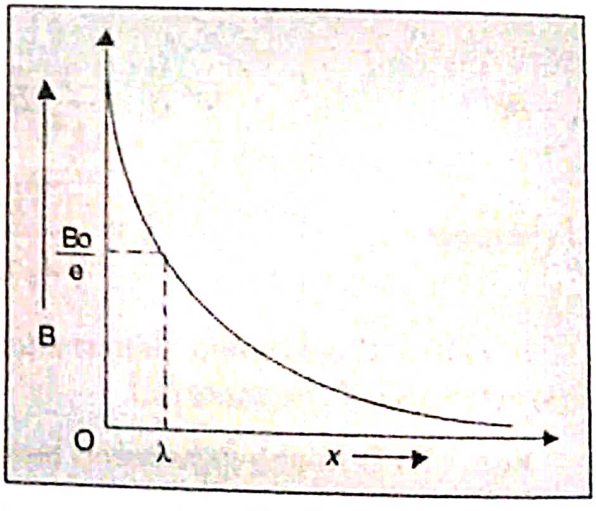


Fig (7.8)

7.8 PENETRATION DEPTH

We know that flux density inside a super conductor changes as

$$B = B_0 e^{-x/\lambda}$$

using eqn. (7.19)

If we put $x = \lambda$

Then $B = B_0 e^{-1}$

or $B = \frac{B_0}{e}$

Thus penetration depth is defined as the distance from surface of the superconductor at which the magnetic flux density decays to $\frac{1}{e}$ of its value at the surface of superconductor. It is given as

$$\lambda(0) = \sqrt{\frac{m}{\mu_0 n_s e^2}} \qquad \text{(at temperature } 0K\text{)}$$

Since λ contains n_s which varies with temperature. Thus penetration depth is a function of temperature of the sample.

For $T > T_c, \quad n_s = 0$

At $T = 0, \quad n_s = \text{maximum}$

$\therefore \quad \lambda = \text{minimum}$

Thus in general λ increases with increase of temperature of the sample.

The empirical relation between λ and temperature (T) is

$$\lambda(T) = \frac{\lambda(0)}{\left[1 - \left(\frac{T}{T_c}\right)^4\right]^{1/2}} \qquad \ldots(7.21)$$

where $\lambda(0)$ is penetration depth at $0K$ and $\lambda(T)$ is penetration depth at TK.

Eqn. (7.21) can be written as

$$\left[\frac{\lambda(T)}{\lambda(0)}\right]^2 = \left[1 - \left(\frac{T}{T_c}\right)^4\right]^{-1} \qquad \ldots(7.22)$$

The variation of λ with T is shown in Fig. (7.9). Equation (7.19) implies that super conducting electron density is given as

$$n_s = n_0 \left[1 - \left(\frac{T}{T_c}\right)^4\right] \qquad \ldots(7.23)$$

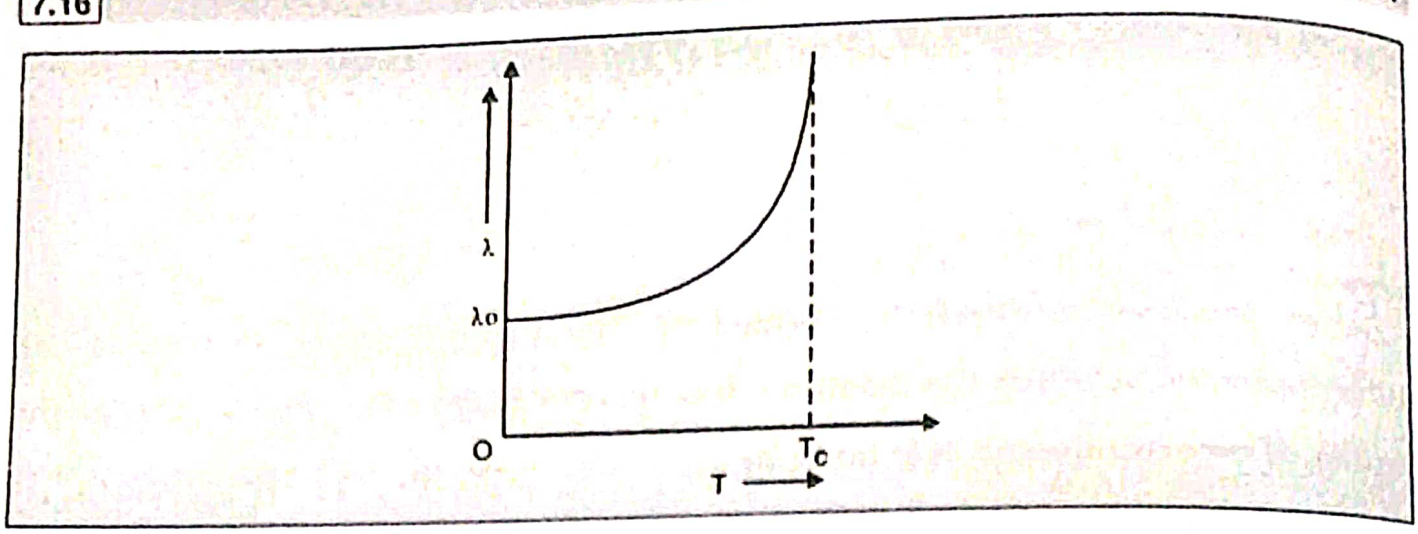


Fig. (7.9)

The density of superconducting electrons increases from zero at T_c to n_0 at $T = 0K$ as shown in Fig. (7.10)

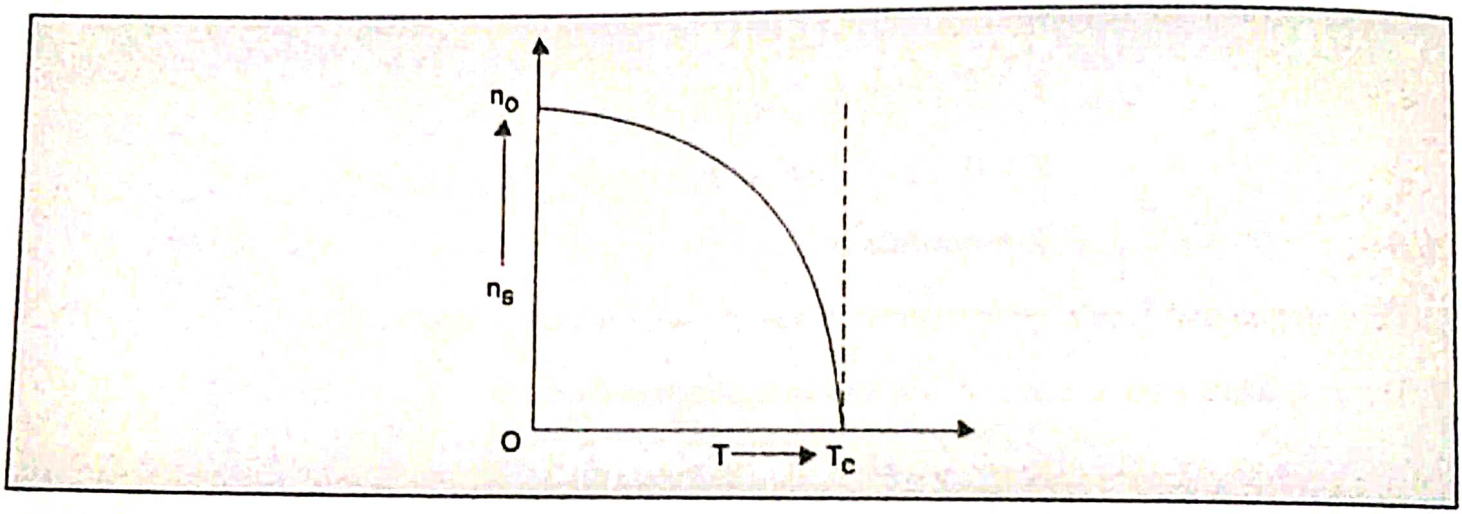


Fig. (7.10)

From eqn. (7.23)

$$\frac{n_0}{n_s} = \left[1 - \left(\frac{T}{T_c}\right)^4\right]^{-1} \qquad \ldots(7.24)$$

From eqns. (7.22 & 7.24)

$$\left[\frac{\lambda(T)}{\lambda(0)}\right]^2 = \frac{n_0}{n_s}$$

$$\therefore \qquad \lambda(T) = \lambda(0)\left(\frac{n_0}{n_s}\right)^{1/2}$$

7.9 ISOTOPE EFFECT

It is observed that the critical temperature of superconductors decreases with increasing isotopic mass M. It is given by

$$T_c \propto \frac{1}{\sqrt{M}}$$

or $$T_c\sqrt{M} = \text{constant} \qquad \ldots(7.25)$$

The variation of critical temperature of an element with its isotopic mass is known as isotopic effect.

The variation of T_c with $\frac{1}{\sqrt{M}}$ is shown in Fig (7.11).

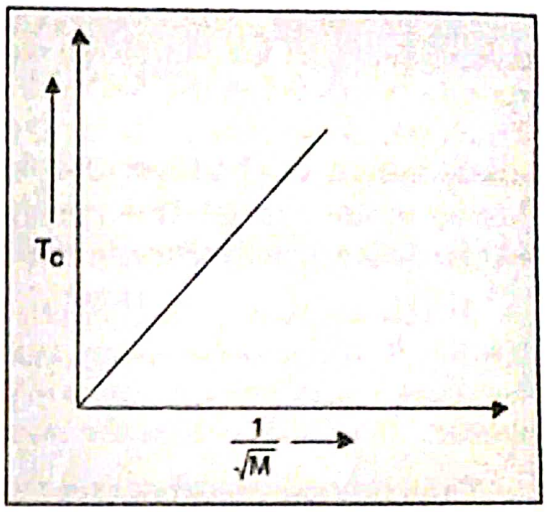


Fig. (7.11)

This effect was discovered by Maxwell and Reynolds *i.e.* as average isotopic mass of mercury varies from 199.5 to 203.4 amu, the value of T_c changes from 4.185 to 4.146 K where T_c is critical temperature in Kelvin. Experimentally it was found that M and T_c satisfy the empirical relation $T_c\sqrt{M}$ = constant.

Let T_0 = Debye temperature for the specimen. It is that temperature above which specific heat of solid becomes constant *i.e.* Dulong and Petal law is obeyed.

Debye temperature (T_D) is related to critical temperature by equation

$$T_D\sqrt{M} = \text{constant} \qquad \ldots(7.26)$$

Dividing eqn. (7.25) by eqn. (7.26), we get

$$\frac{T_c}{T_D} = \text{constant}$$

Thus T_c depends on T_D. Since T_D depends on speed of sound in that solid and speed of sound in a solid is determined by lattice vibrations. Thus above relation suggests that lattice vibrations must have some relation with superconductivity. Hence electron lattice interactions must be taken into account in finding explanation of superconductivity. When a superconductor undergoes transition from normal state to super conducting state, there is sudden change in manner in which the current flows. This transition occurs at critical temperature T_c. The dependence of T_c on the isotopic mass M has been experimentally confirmed.

The dependence of T_c on M is given by

$$T_c \propto M^{-\beta}$$

where β varies from 0 (Rubidium) to 0.5 (Cadmium) called isotopic effect coefficient.

7.10 BCS THEORY

The quantum theory of superconductivity was given by Bardeen, Copper and Schrieffer in 1957, which is known as BCS theory. This theory is based on the formation of **Cooper pairs.**

The electrical resistance in metals arises due to collision of conduction electrons (*i.e.* free electrons) with vibrating ions of the lattice. In normal state the force between the electrons is repulsive. But in super conducting state, the force between two electrons become attractive due to formation of cooper pair. The BCS theory is briefly discussed below.

The electron-phonon interaction is the basis of BCS theory. As we have already discussed in isotopic effect that lattice vibrations (phonons) play an important role in the theory of superconductivity and current carrying electrons in superconductor do not move independently of ion lattice but somehow are interacting with the lattice. When an electron approaches an ion in the lattice, both interact electrostatically (*i.e.* Coulomb attraction takes place). Thus momentum is imparted to ions which causes them to move together due to elastic behavior of lattice. This slight movement together increases the positive charge density in the region. This region of increased positive charge density propagates a wave, which carries a momentum through lattice.

At this stage, if another electron passes by the moving region of increased positive charge density, it will experience an attractive coulomb interaction and hence can absorb all the momentum, the moving region carries. In other words the second electron can absorb the phonon, thereby absorbing the momentum supplied by the first electron.

Thus two electrons have exchanged momentum through an interaction involving phonon as intermediary. In this way interaction between two electrons take place. This is an attractive interaction because at each step electrons participate in attractive way. This interaction between two electrons via phonon exceeds the coulomb repulsion. The pair of these two electrons is known as **Cooper pairs.** The above discussion can be depicted in quantum mechanical terms. As shown in Fig (7.12) first electron of wave vector $\vec{K}$ (because momentum $\vec{p} = \hbar\vec{K}$) emits a photon $\vec{q}$, which is absorbed by second electron with wave vector $\vec{K}'$. This scatters $\vec{K}$ into $\vec{K} - \vec{q}$ and $\vec{K}'$ into $\vec{K}' + \vec{q}$. The whole process is virtual and the phonons involved are known as virtual phonons, because of very short life of these phonons the energy may not be conserved (which is in accordance with uncertain principle).

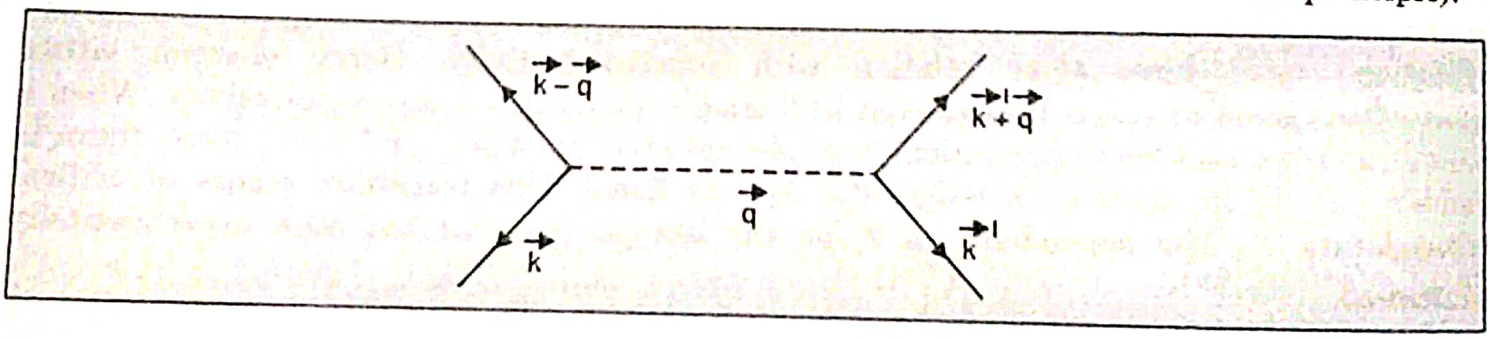


Fig. (7.12)

Thus lattice vibrations play an important role in the phenomenon of superconductivity. Hence materials with large amplitude lattice vibrations are good superconductors, though they may not be good conductors at room temperature. Good conductors such as copper, silver etc. have small amplitude lattice vibrations, hence they are not superconductors. Metals like mercury, tin, lead etc. have large amplitude lattice vibrations, hence they are good superconductors. The electrons in the cooper pair have opposite spins, so the pair has a total zero spin. As a result, the electron pairs in superconductors are **bosons.** Energy of cooper pair is lower than the energy of two individual electrons.

The cooper pair of electrons moves on without suffering any deviation either by impurities or thermal vibration. Hence there is no exchange of energy between pair of electrons and lattice ions. If an electric field is established inside the substance, the electrons gain additional kinetic energy and give rise to a current. The pair of electrons does not transfer any energy to the lattice. Therefore, they do not get slowed down. As a consequence of this, the substance does not possess any electrical resistivity and the conduction is large. **Thus when the pair of electrons flows in the form of cooper pair, they do not encounter any scattering and the resistance vanishes i.e. conductivity becomes infinity which is named as superconductivity.**

In case of superconductivity the electrons interact with each other attractively and phonons mediate this interaction. This interacting Fermi gas forms the BCS ground state. This ground state is separated from lowest excited state by energy-gap E_g, which is the binding energy of cooper pair. The energy gap in super conducting state occurs at $0K$, which pairing is complete and vanishes at $T = T_c$, where pairing also vanishes.

The energy gap E_g of a superconductor at $0K$ is given by the formula

$$E_g(0) \approx 3.53\, kT_c$$

where k is Boltzman's constant and T_c is the critical temperature of a superconductor.

7.11 APPLICATIONS OF SUPERCONDUCTORS

Following are some main applications of superconductivity :

(I) Magnets :

(i) Hard superconducting (type-II) materials are used for making very strong magnets of about 50 Tesla. They consume small energy at high magnetic field strength as compared to conventional copper solenoid.

(ii) They are used in Nuclear Magnetic Resonance (NMR) medical diagnostic and spectroscopy.

(iii) They are used in magnetic shielding.

(iv) They are used in magnetic levitation.

(II) Energy-Related

(i) They are used in production by magnetic fusion and magneto-hydrodynamics.

(ii) Energy storage (magnetic).

(iii) Electric power transmission.

(III) Temperature : They are used in

(i) High speed trains

(ii) Ship drive system

(IV) Electronic and Small Devices : They are used in

(i) Bolometer

(ii) Electromagnetic shielding

(iii) SQUIDS (Super-conducting Quantum Interference Devices)

(V) Computers and Information Processing

(i) Semiconductor-superconductor hybrids

(ii) FETs

(iii) Voltage standard

(iv) Matched filters

SOLVED PROBLEMS

PROBLEM 1. Calculate the superconducting electron density of mercury at 3.5 K. Given transition temperature of mercury is 4.22 K.

Solution

The normal current density in mercury can be found in terms of molecular weight and density. Therefore

$$n_0 = \frac{N\rho}{M} = \frac{6.023 \times 10^{26} \times 13.55 \times 10^3}{200.6}$$

$$= 4.06 \times 10^{28}/m^3$$

$$n_s = n_0\left[1 - \left(\frac{T}{T_c}\right)^4\right] = 4.06 \times 10^{28}\left[1 - \frac{(3.5)^4}{(4.22)^4}\right]$$

$$= 2.138 \times 10^{28}/m^3$$

PROBLEM 2. The critical temperature T_c for H_g with isotopic mass 199.5 is 4.185 K. Calculate its critical temperature, when isotopic mass changes to 203.4.

Solution

Here, $T_{c_1} = 4.185K$, $T_{c_2} = ?$

$M_1 = 199.5$, $M_2 = 203.4$

We know that

$$T_c\sqrt{M} = \text{constant}$$

$$\therefore \quad \frac{T_{c_1}}{T_{c_2}} = \sqrt{\frac{M_2}{M_1}}$$

or $$T_{c_2} = T_{c_1}\sqrt{\frac{M_1}{M_2}}$$

$$= 4.185\sqrt{\frac{199.5}{203.4}} = 4.14\ K$$

PROBLEM 3. A super conducting lead has critical temperature of 7.26K at zero magnetic field and at 0K the critical field is 8×10^5 A/m. Find the critical field at 5.5 K.

Solution

Here, $H_c(0) = 8 \times 10^5\ A/m$, $T_c = 7.26\ K$

$T = 5.5\ K$

$$H_c = H_c(0)\left[1 - \left(\frac{T}{T_c}\right)^2\right]$$

or $$H_c = 8 \times 10^5\left[1 - \left(\frac{5.5}{7.26}\right)^2\right] = 8 \times 10^5\left[1 - (0.757)^2\right]$$

$$= 8 \times 10^5[1 - 0.573] = 8 \times 10^5[0.427]$$

$$= 3.42 \times 10^5\ A/m$$

PROBLEM 4. Calculate the critical current, which can flow through a long thin superconducting wire of diameter 10^{-4} m. The critical field of aluminium is 7.9×10^3 A/m.

Solution

Here, $d = 10^{-4}\ m$ or $r = \frac{d}{2} = \frac{10^{-4}}{2} = 0.5 \times 10^{-4}\ m$

$$H_c = 7.9 \times 10^3\ A/m$$

$$I_c = 2\pi r\, H_c = 2 \times 3.14 \times 0.5 \times 10^{-4} \times 7.9 \times 10^3$$

$$= 24.81 \times 10^{-1} = 2.48\ A$$

PROBLEM 5. The transition temperature of lead is 7.2 K. However it loses the superconducting property if subjected to a magnetic field of 3.3×10^4 A/m at 5K. Find the value of H_c (0) which will allow the metal to retain its superconductivity at 0K.

Solution

Here, $T_c = 7.2K$, $T = 5K$

$$H_c = 3.3 \times 10^4\ A/m$$

$$H_c = H_c(0)\left[1 - \frac{T^2}{T_c^2}\right]$$

$$H_c(0) = \frac{H_c}{\left[1 - \left(\frac{T}{T_c}\right)^2\right]}$$

$$= \frac{3.3 \times 10^4}{\left[1 - \left(\frac{5}{7.2}\right)^2\right]} = \frac{3.3 \times 10^4}{\left[1 - \left(\frac{25}{51.28}\right)\right]}$$

$$= \frac{3.3 \times 10^4}{(1 - 0.487)} = \frac{3.3 \times 10^4}{0.513}$$

$$= 6.43 \times 10^4 \, A/m$$

PROBLEM 6. The critical fields of a superconducting alloy at temperature $6K$ and $8K$ are 76×10^5 A/m and 43×10^5 A/m. Find critical temperature.

Solution

Here, $T_1 = 6K$, $T_2 = 8K$

$H_c(T_1) = 76 \times 10^5 \, A/m$

$H_c(T_2) = 43 \times 10^5 \, A/m$

We know that

$$H_c(T) = H_c(0)\left[1 - \left(\frac{T}{T_c}\right)^2\right] = H_c(0)\left(\frac{T_c^2 - T^2}{T_c^2}\right)$$

$$\therefore \quad \frac{H_c(T_1)}{H_c(T_2)} = \frac{T_c^2 - T_1^2}{T_c^2 - T_2^2}$$

$$\frac{76 \times 10^5}{43 \times 10^5} = \frac{T_c^2 - 36}{T_c^2 - 64}$$

$$\frac{76}{43} = \frac{T_c^2 - 36}{T_c^2 - 64}$$

$$76\,T_c^2 - 4864 = 43\,T_c^2 - 1548$$

$$76\,T_c^2 - 43\,T_c^2 = 4864 - 1548$$

$$33\,T_c^2 = 3316$$

$$T_c^2 = \frac{3316}{33} = 100.48$$

$$\therefore \quad T_c = 10.02 \, K$$

PROBLEM 7. Calculate the critical current density for 1 mm diameter of wire at 4.2 K. Assume the critical magnetic field intensity depends on temperature (T). Given T_c for lead is 7.18 K and H_c (0) for lead is 6.5×10^4 A/m.

Solution

Here, $T = 4.2\ K,\ T_c = 7.18\ K$

$H_c(0) = 6.5 \times 10^4\ A/m,\ d = 1\ mm = 10^{-3}\ m$

or $r = 0.5 \times 10^{-3}\ m$

$$H_c(T) = H_c(0)\left[1 - \frac{T^2}{T_c^2}\right] = 6.5 \times 10^4\left[1 - \frac{(4.2)^2}{(7.18)^2}\right]$$

$$= 6.5 \times 10^4\left[\frac{(7.18)^2 - (4.2)^2}{(7.18)^2}\right] = 4.28 \times 10^4\ A/m$$

$$\therefore\ I_c = 2\pi r\, H_c = 2 \times 3.14 \times 0.5 \times 10^{-3} \times 4.28 \times 10^4$$

$$= 13.44 \times 10 = 134.4\ A$$

$$J_c = \frac{I_c}{A} = \frac{I_c}{\pi r^2} = \frac{134.4}{3.14 \times (5 \times 10^{-4})^2} = \frac{134.4}{3.14 \times 25} \times 10^8$$

$$= \frac{134.4}{78.5} \times 10^8 = 1.71 \times 10^8\ A/m^2$$

PROBLEM 8. **The London penetration depth for a sample at 6K at 7K are 41.2 nm and 180.3 nm respectively. Calculate its transition temperature as well as the penetration depth at 0K.**

Solution

Here, $T_1 = 6K,\ T_2 = 7K$

$\lambda(T_1) = 41.2\ nm = 41.2 \times 10^{-9}\ m$

$\lambda(T_2) = 180.2\ nm = 180.3 \times 10^{-9}\ m$

We know that

$$\lambda(T) = \frac{\lambda(0)}{\sqrt{1 - \left(\frac{T}{T_c}\right)^4}}$$

$$\therefore\ \frac{\lambda(T_1)}{\lambda(T_2)} = \frac{\sqrt{1 - \left(\frac{T_2}{T_c}\right)^4}}{\sqrt{1 - \left(\frac{T_1}{T_c}\right)^4}} = \sqrt{\frac{T_c^4 - T_2^4}{T_c^4 - T_1^4}}$$

$$\text{or}\quad \left[\frac{\lambda(T_1)}{\lambda(T_2)}\right]^2 = \frac{T_c^4 - T_2^4}{T_c^4 - T_1^4}$$

$$\text{or} \left[\frac{41.2 \times 10^{-9}}{180.3 \times 10^{-9}}\right]^2 = \frac{T_c^4 - (7)^4}{T_c^4 - (6)^4}$$

$$\text{or} \left[\frac{41.2}{180.3}\right]^2 = \frac{T_c^4 - 2401}{T_c^4 - 1296}$$

$$\text{or} \left[\frac{180.3}{41.2}\right]^2 = \frac{T_c^4 - 1296}{T_c^4 - 2401}$$

$$\therefore \quad (4.376)^2 = \frac{T_c^2 - 1296}{T_c^4 - 2401}$$

$$\frac{19.15}{1} = \frac{T_c^4 - 1296}{T_c^4 - 2401}$$

$$\text{or} \quad 19.15\, T_c^4 - 45979.15 = T_c^4 - 1296$$

$$19.15\, T_c^4 - T_c^4 = 45979.15 - 1296$$

$$18.15\, T_c^4 = 44683.15$$

$$T_c^4 = \frac{44683.15}{18.15} = 2461.88$$

$$\therefore \quad T_c = 7.04\ K$$

$$\therefore \quad \lambda(6) = \frac{\lambda(0)}{\sqrt{1 - \left(\frac{6}{T_c}\right)^4}}$$

$$\lambda(0) = \lambda(6) \sqrt{1 - \left(\frac{6}{7.04}\right)^4}$$

$$= 41.2 \times 10^{-9} \sqrt{1 - \frac{1296}{2461.88}}$$

$$= 41.2 \times 10^{-9} \sqrt{1 - 0.5264}$$

$$= 41.2 \times 10^{-9} \sqrt{0.4734}$$

$$= 41.2 \times 10^{-9} \times 0.688$$

$$= 28.34 \times 10^{-9}\ m = 28.34\ nm$$

PROBLEM 9. **Calculate the value of London penetration depth λ_0 at 0K for lead, whose density is 11.3 × 10^3 kg/m^3 and atomic weight is 207.19. Its T_c is 7.22 K. Calculate the increase in λ at 3.61 K from its value at 0K.**

Solution

Here, $T_c = 7.22\ K,\ T = 3.61\ K,\ \rho = 11.3 \times 10^3\ kg/m^3$

$$n = \frac{N}{V} = \frac{N_0 \rho}{W}$$

$$= \frac{6.02 \times 10^{26} \times 11.3 \times 10^3}{207.19} = 3.29 \times 10^{28}/m^3$$

$$\lambda_0 = \left[\frac{m}{\mu_0 n e^2}\right]^{1/2}$$

$$= \left[\frac{9.1 \times 10^{-31}}{4\pi \times 10^{-7} \times 3.29 \times 10^{28} \times (1.6 \times 10^{-19})^2}\right]^{1/2}$$

$$= 2.93 \times 10^{-9}\ m = 29.3\ nm$$

$$\lambda(T) = \lambda_0 \left[1 - \left(\frac{T}{T_c}\right)^4\right]^{-1/2}$$

$$= 29.3 \left[1 - \left(\frac{3.61}{7.23}\right)^4\right]^{-1/2}$$

$$= 30.29\ nm$$

Increase in penetration depth

$$= \frac{30.26 - 29.3}{29.3} = 0.03276 = 32.76\%$$

PROBLEM 10. **Calculate the energy gap for tin (*Sn*), whose critical temperature is 3.72 *K*.**

Solution

Here, $T_c = 3.72\ K,\ k = 1.38 \times 10^{-23}\ J/K$

$$E_g = 3.53\ k\ T_c$$

$$= 3.53 \times 1.38 \times 10^{-23} \times 3.72$$

$$= 1.18 \times 10^{-22}\ \text{Joule}$$

$$= \frac{1.18 \times 10^{-22}}{1.6 \times 10^{-19}}\ eV = 1.13 \times 10^{-3}\ eV$$

CONCEPTUAL QUESTIONS

Q. 1. What is a superconductor ?

Ans. There are certain metals and alloys when cooled to sufficient low temperature exhibit almost zero resistivity. This phenomenon is called superconductivity and the substance is called superconductor.

Q. 2. What factors can affect the superconducting behaviour of a superconductor ?

Ans. The superconducting behaviour can be affected by (i) temperature of the substance (ii) the magnetic field applied across the substance (iii) the current passed through it.

Q. 3. What are the conditions for a material to be a superconductor ?

Ans. Following are the conditions for a material to be a superconductor :

(i) The material must be cooled below the characteristic temperature, known as its superconducting transition or critical temperature (T_c).

(ii) The magnetic field to which the material exposed must be below the characteristic value, known as critical magnetic field (H_c).

(iii) The current passing through a given cross-section of the material must be below a characteristic level, known as the critical current density (J_c).

Q. 4. What is the effect of magnetic field on superconductivity ?

Ans. The effect of magnetic field on superconductivity is that, the superconductivity can be destroyed by application of magnetic field greater than critical value. The minimum magnetic field necessary to destroy the superconductivity and to restore the normal resistivity is called critical field (H_c).

Q. 5. What is critical temperature of a superconductor ?

Ans. The temperature at which the normal metal passes into superconducting state is called transition temperature or critical temperature (T_c).

Q. 6. Name few properties which do not change in superconducting transitions.

Ans. Following are the properties which do not change in superconducting transitions (i) X-ray diffraction pattern (ii) reflectivity (iii) absorption of slow and fast electrons (iv) elastic properties and (v) thermal properties.

Q. 7. Name few properties which change in super conducting transitions.

Ans. Following are some of the properties which change in superconducting transitions.

(i) electrical properties (resistance) (ii) magnetic properties (iii) specific heat (iv) thermoelectric effects and (v) thermal conductivity.

Q. 8. What is Silsbee effect ?

Ans. When a strong current is passed through the superconductor, the magnetism produced in the specimen destroys its conductivity. The cause of destruction of superconductivity is the magnetic field associated with the current and not the

current itself. Thus Silsbee effect poses a limit to the current to be passed through a superconductor.

Q. 9. What is isotope effect in superconductivity ?

Ans. The variation of critical temperature (T_c) of an element with its isotopic mass (M) is known as isotope effect.

i.e. $$T_c \propto \frac{1}{\sqrt{M}}$$

or $$T_c\sqrt{M} = \text{constant}$$

Q. 10. What is Meissner's effect ?

Ans. A super conducting material kept in a magnetic field expels the magnetic flux out of its body when it is cooled below the critical temperature and thus becomes perfect diamagnet. This effect is called Meissner's effect.

Q. 11. What are Cooper pairs ?

Ans. Cooper pair is a bound pair of electrons formed by the interaction between the electrons with opposite spin and momenta in a phonon field.

Q. 12. What should be two distinct properties of a material to be superconductor ?

Ans. (i) Zero resistivity or infinite conductivity and (ii) $B = 0$ inside the superconductor.

Q. 13. Why type-II superconductors are more important ?

Ans. Type-II superconductors (or hard superconductors) can carry high current densities, as a result they have great technological values.

Q. 14. What are type-I superconductors ?

Ans. Type-I superconductor is one in which the transition from superconducting state to normal state in the presence of magnetic field occurs sharply at the critical value H_c. Type-I superconductors are ideal diamagnetics.

Q. 15. What are type-II superconductors ?

Ans. Type-II superconductors are characterized by two magnetic fields H_{c_1} and H_{c_2}. Between H_{c_1} and H_{c_2} the specimen is in mixed state. Above H_{c_2} the specimen is in normal conductor.

Q. 16. Give the main characteristics of a cooper pair.

Ans. When the electrons flow in the form of cooper pairs in materials, they do not encounter any scattering and resistance factor vanishes (*i.e.* conductivity becomes infinity), which is named as superconductivity.

Q. 17. Why are type-I superconductors poor current carrying conductors ?

Ans. In Type-I superconductors the magnetic field can penetrate only the surface layer and current can flow in this layer. The resistance increases from zero to some value as in the case of a normal conductor. Consequently type-I superconductors are poor carriers of electric current.

Q. 18. Why good conductors are not superconductors ?

Ans. Lattice vibrations play an important role in the phenomenon of superconductivity, hence materials with large amplitude lattice vibrations are good superconductors, though they may not be good conductors at room temperature. Good conductors such as copper, silver etc. have small amplitude lattice vibrations, hence they are not superconductors.

Q. 19. Define the penetration depth.

Ans. The penetration depth can be defined as the perpendicular distance from the surface of a superconductor to a point inside, where superconducting density is $\frac{1}{e}$ times of its value on the surface.

Also it is defined as the distance inside the superconductor at which magnetic field falls to $\left(\frac{1}{e}\right)$ times the magnetic field at the surface.

Q. 20. What are SQUIDS ?

Ans. SQUID stands for **superconducting quantum interference device.** It is a superconducting loop with a weak link to measure magnetic flux changes within the loop. SQUID instruments used to study tiny magnetic signals in the brain. SQUID magnetometers are used to detect paramagnetic response in liver, giving to doctors an accurate read out of iron in the body. They can measure the feeble magnetic fields of the order of 10^{-14} to 10^{-15} Tesla which are produced by electrical currents in heart and brain.

MULTIPLE CHOICE QUESTIONS

Choose the correct alternative for each question given below :

1. **Superconductivity was first discovered by :**
   (a) Meissner and Ochsenfeld (b) C.H. Townes
   (c) Heike Kamerlingh Onnes (d) C.A. Reynolds
2. **The metal mercury becomes superconductor at :**
   (a) 4.15 K (b) 4.15°C
   (c) 4.15 F (d) 4.15 R
3. **Superconductors are perfect :**
   (a) Diamagnetic materials (b) Ferromagnetic materials
   (c) Antiferromagnetic materials (d) Paramagnetic materials
4. **A superconductor has :**
   (a) Zero conductivity (b) Infinite resistivity
   (c) Infinite conductivity (d) None of the above

5. **The resistivity of a pure superconductor at transition temperature :**
   (a) gradually reaches zero
   (b) oscillates and become zero
   (c) suddenly becomes zero
   (d) none of these.

6. **The transition temperature of a superconductor :**
   (a) depends on isotopic mass
   (b) does not depend on isotopic mass
   (c) independent of everything
   (d) none of these.

7. **For superconductors, which of the following statement is false :**
   (a) All thermoelectric effect disappear in super conducting state
   (b) Magnetic susceptibility of superconductor is zero
   (c) Heating loss in superconductor is zero
   (d) At critical temperature (T_c) the critical field is zero.

8. **Magnetic susceptibility of superconductors is given by**
   (a) $\chi = -1$
   (b) $\chi = 0$
   (c) $\chi = 1$
   (d) $\chi >> 1$

9. **The temperature at which a metal becomes superconducting is called :**
   (a) Neel's temperature
   (b) Curie's temperature
   (c) Meissner point
   (d) Transition temperature

10. **The critical field strength of a superconductor :**
    (a) depends on mechanical stress
    (b) depends on the purity of the metal
    (c) varies with temperature
    (d) all the above

11. **A superconducting material when placed in a magnetic field will :**
    (a) Attract the magnetic field towards sits centre.
    (b) Repel all the magnetic lines of force passing through it.
    (c) Attract the magnetic field but transfer it into a concentrated zone.
    (d) Not influence the magnetic field.

12. **Superconductivity is usually exhibited at :**
    (a) Low temperatures
    (b) High temperatures
    (c) Very high temperatures
    (d) High temperatures

13. **Which of the property is not exhibited by superconductors :**
    (a) $\mu_r = 0$
    (b) Copper loss = 0
    (c) $B \neq 0$
    (d) $\chi = -1$

14. **According to isotope effect, the transition temperature (T_c) for superconductor is proportional to :**
    (a) $M^{-1/2}$
    (b) $M^{-1/4}$
    (c) $\sqrt{M}$
    (d) $-\frac{1}{M}$.

15. As isotopic mass of mercury decreases to one-fourth. Its T_c will become:
(a) Half
(b) one-fourth
(c) Remains same
(d) Double

16. BCS theory is an attempt to explain :
(a) Magnetism
(b) Superconductivity
(c) Thermo-electric effect
(d) Heating effect

17. In a particular superconductor, transition takes place gradually, it belongs to :
(a) Type-I
(b) Type-II
(c) Type-I and Type II both
(d) none of the above

18. Hard superconductors observe :
(a) break down of Silsbee's rule
(b) Incomplete Meissner effect
(c) high critical field and transition
(d) all the above

19. BCS theory is valid for :
(a) low temperature superconductors
(b) high temperature superconductors
(c) both low and high temperature superconductors
(d) neither low nor high temperature superconductors

20. The isotopic effect coefficient for superconductors varies from (is) :
(a) 0 – 0.3
(b) 0.45 – 0.50
(c) 1 – 2
(d) Unity

21. The cooper pairs are :
(a) Bose-Einstein particles (or Bosons)
(b) Fermi-Dirac particles (or Fermions)
(c) Classical particles
(d) Electron-positron pairs

22. The London penetration depth is given by

(a) $\lambda = \left(\frac{m}{\mu_0 n_s e^2}\right)^{1/2}$

(b) $\lambda = \left(\frac{n_s}{m\,\mu_0 e^2}\right)^{1/2}$

(c) $\lambda = (n_s m \mu_0 e^2)^{1/2}$

(d) $\lambda = \left(\frac{\mu_0}{m n_s e^2}\right)^{1/2}$

Answers

1.	(c)	2.	(a)	3.	(a)	4.	(c)	5.	(c)
6.	(a)	7.	(b)	8.	(a)	9.	(d)	10	(d)
11.	(b)	12.	(a)	13.	(c)	14.	(a)	15.	(d)
16.	(b)	17.	(b)	18.	(d)	19.	(a)	20.	(b)
21.	(a)	22.	(a)						

CHAPTER AT A GLANCE

1. **Superconductivity :** The phenomena in which the electrical resistance of a substance drops suddenly to zero when it is cooled below a certain temperature.

2. **Critical Temperature :** The temperature at which the normal metal state passes into super conducting state is called transition temperature or critical temperature (T_c).

3. There are certain properties which do not change in super conducting transitions *i.e.* X-ray diffraction pattern of a crystal, reflectivity, absorption of slow or fast electrons, elastic and thermal properties etc.

4. There are certain properties which change in super conducting transitions *i.e.* electrical properties (resistance) of material, magnetic properties, specific heat, thermoelectric effects and thermal conductivity etc.

5. **Critical Magnetic Field :** The minimum applied magnetic field necessary to destroy superconductivity and restore the normal resistivity is called critical magnetic field (H_c).

   Critical magnetic field varies with temperature as

$$H_c = H_0\left(1 - \frac{T^2}{T_c^2}\right)$$

   where H_0 is critical magnetic field at $0K$, H_c is critical magnetic field at temperature T and T_c is critical temperature.

6. **Silsbee Rule** is given as

$$H_c = \frac{I_c}{2\pi r}$$

   where I_c is critical current, H_c is critical magnetic field and r is radius of wire.

7. **Meissner Effect :** Meissner found that if a superconductor is cooled in a magnetic field, below critical temperature corresponding to that field then the lines of magnetic induction are expelled from the material at the transition. This effect is called Meissner effect.

8. **Type-I Superconductor** is one in which the transition from superconducting state to normal state in the presence of magnetic field occurs sharply at the critical value H_c. Type-I superconductors are ideal diamagnetics.

9. **Type-II Superconductors** are characterized by two critical fields, H_{c_1} and H_{c_2}. Between H_{c_1} and H_{c_2} the specimen is in mixed state. Above H_{c_2} the specimen is normal conductor.

10. According to London, a superconductor state is supposed to be formed by both normal and super conducting electrons. The **First London Equation** is

$$\frac{d\vec{J}_s}{dt} = \frac{n_s e^2}{m}\vec{E}$$

and **Second London Equation is**

$$\vec{J}_s = -\frac{n_s e^2}{m}\vec{A}$$

where notations have their usual meanings.

11. **London penetration** depth is defined as the distance inside the superconductor at which magnetic field falls to $\left(\frac{1}{e}\right)$ times the magnetic field at the surface.

12. The temperature dependence of penetration depth $\lambda(T)$ is given by

$$\left[\frac{\lambda(T)}{\lambda(0)}\right]^2 = \left[1-\left(\frac{T}{T_c}\right)^4\right]^{-1}$$

where $$\lambda(0) = \left(\frac{m_0}{\mu_0 n_s e^2}\right)^{1/2}$$

13. The variation of critical temperature of an element with its isotopic mass is known as isotope effect *i.e.*

$$T_c \propto \frac{1}{\sqrt{M}} \quad \text{or} \quad T_c\sqrt{M} = \text{constant}$$

14. BCS theory explains successfully almost all phenomena associated with superconductivity.

15. Cooper pair is a bound pair of electrons formed by the interaction between electrons in a phonon field.

16. According to BCS theory, when a pair of electrons in the form of Cooper-pairs flow, the pairs do not encounter any scattering in the material and resistance factor vanishes *i.e.* conductivity becomes infinity, which is named as superconductivity.

SHORT ANSWER QUESTIONS

1. What is superconductivity ?
2. Superconductors are perfectly diamagnetic in nature, why ?
3. Why superconductors are perfectly diamagnetic in nature ?
4. What is Meissner effect ?
5. Differentiate between Type-I and Type-II superconductors.
6. Plot the graphs for Type-I and Type-II superconductors.
7. Define critical temperature.

8. What is critical magnetic field?
9. Explain briefly the formation of cooper pairs.
10. Write a short note on BCS theory.
11. Write a short note on applications of superconductivity.
12. Define London penetration depth and write its expressions.
13. What are cooper pairs ?
14. What is isotope effect ?
15. Why good conductors are not superconductors?

LONG ANSWER QUESTIONS

1. What is superconductivity ? Discuss the temperature dependence of resistivity in superconducting material.
2. Define superconductors. What are the properties of superconductors ?
3. What is superconductivity ? What are the properties which do not change in superconducting transitions ?
4. Define superconductors. What are the properties which change in superconducting transition ?
5. What is critical magnetic field ? How it varies with temperature ? Explain Silsbee effect.
6. Define critical magnetic field. Explain the variation of critical magnetic field with temperature. What is Silsbee effect ?
7. What is Meissner effect ? Prove that Meissner effect and the disappearance of resistivity in a superconductor are mutually consistent.
8. State and explain Meissner effect.
9. What do you mean by Meissner effect ? Explain how Meissner effect proves the superconductivity to perfect diamagnetism ?
10. Describe Type-I and Type-II superconductors. Why are Type-I superconductors poor current carrying conductors?
11. What are Type-I and Type-II superconductors ? Explain.
12. Write short notes on : Type-I and Type-II superconductors.
13. What are Type-I and Type-II superconductors ? Distinguish between them.
14. Prove the London equation $\nabla^2 \vec{B} = \frac{1}{\lambda^2} \vec{B}$, where λ is the London penetration depth.
15. Derive London equation and discuss how its solution leads to Meissner effect.
16. Outline some experimental facts about superconductivity.
17. Derive first London equation and give its physical significance.

18. Calculate the expression of penetration depth in superconductors.
19. What are London's equations ? Find the expression for the penetration depth of a superconductor.
20. Explain briefly BCS theory of superconductors.
21. Explain BCS theory of superconductors.
22. What is BCS theory of superconductors ? Write its salient features.
23. What is isotope effect in superconductors ? How it provide a clue to the microscopic BCS theory of superconductivity ?

UNSOLVED NUMERICAL PROBLEMS

1. The critical temperature for a metal with isotopic mass 199.5 is 4.185 K. Calculate the isotopic mass if the critical temperature falls to 4.133 K. [Ans. 204.72]

[Hints : $T_{c_1} M_1^{1/2} = T_{c_2} M_2^{1/2}$ or $M_2^{1/2} = \dfrac{T_{c_1} M_1^{1/2}}{T_{c_2}}$,

$$M_2 = \left(\frac{T_{c_1}}{T_{c_2}}\right)^2 M_1 = \left(\frac{4.185}{4.133}\right)^2 \times 199.5 = (1.013)^2 \times 199.5 = 204.72]$$

2. The isotopes of lead of atomic mass 206 and 210 have T_c values 7.193 K and 7.125 K respectively. Calculate the values of β. [Ans. 0.5]

[Hints : $\dfrac{T_{c_1}}{T_{c_2}} = \left(\dfrac{M_1}{M_2}\right)^{-\beta}$, then $\beta = 0.4962 \approx 0.5$]

3. The critical current passing through a long thin superconducting wire of 0.5 mm radius is 22.608 A, calculate the critical magnetic field. [Ans. 7.2×10^3 A/m]

[Hints : $I_c = 2\pi r H_c$ or $H_c = \dfrac{I_c}{2\pi r} = \dfrac{22.608}{2 \times 3.14 \times 0.5 \times 10^{-3}} = 7.2 \times 10^3$ A/m]

4. Compute the critical current through a long thin superconducting wire of radius 0.3 mm. The critical magnetic field is 7 $k\,A/m$. [Ans. 13.19 A]

[Hints : $I_c = 2\pi r\, H_c = 2 \times 3.14 \times 0.3 \times 10^{-3} \times 7 \times 10^3 = 13.19$ A]

5. Transition temperature for Al is 1.8 K. Calculate the energy gap for aluminium.

[Ans. 0.5×10^{-3} eV]

[Hints : $E_g = 3.53\, k\, T_c = \dfrac{3.53 \times 1.38 \times 10^{-23} \times 1.8}{1.6 \times 10^{-19}} = 0.55 \times 10^{-3}$ eV]

6. The transition temperature for H_g is 4.153 K. Calculate the energy gap for H_g.

[Ans. 1.26×10^{-3} eV]

[Hints : $E_g = 3.53\, k\, T_c = \dfrac{3.53 \times 1.38 \times 10^{-23} \times 4.153}{1.6 \times 10^{-19}} = 1.26 \times 10^{-3}$ eV]

7. A super-conducting Sn (Tin) has a critical temperature of 3.7 K has magnetic field of 0.0306 T at $0K$. Find the critical field of $2K$. [Ans. 0.02166 Tesla]

[Hints : $H_c = H_0\left(1 - \dfrac{T^2}{T_c^2}\right) = 0.0306\left[1 - \left(\dfrac{2}{3.7}\right)^2\right] = 0.02166$ Tesla]

8. The critical field for niobium is 1×10^5 A/m at $8K$ and 2×10^5 A/m at $0K$. Calculate critical temperature of the material. [Ans. 11.31 K]

[Hints : $T_c = \dfrac{T}{\left[1 - \dfrac{H_c}{H_0}\right]^{1/2}} = \dfrac{8}{\left[1 - \dfrac{1 \times 10^5}{2 \times 10^5}\right]^{1/2}} = 11.31$ K]

9. The transition temperature for Pb is 7.26 K. The maximum critical field for the material is 8×10^5 A/m. Pb has to be used as superconductor subjected to a magnetic field of 4×10^4 A/m. What precaution will have to be taken?

[Ans. Temp. should be held below 7.08K]

[Hints : $T = T_c\left[1 - \dfrac{H_c}{H_0}\right]^{1/2} = 7.26\left[1 - \dfrac{4 \times 10^4}{8 \times 10^5}\right] = 7.08$ K]

10. For a specimen of superconductor, the critical fields are 1.4×10^5 A/m and 4.2×10^5 A/m respectively for temperature $14K$ and $13K$ respectively. Calculate the transition temperature. [Ans. 14.5 K]

[Hints : $\dfrac{H_{c_2}}{H_{c_1}} = \dfrac{T_c^2 - (13)^2}{T_c^2 - (14)^2}$ or $\dfrac{4.2 \times 10^5}{1.4 \times 10^5} = \dfrac{T_c^2 - (13)^2}{T_c^2 - (14)^2} \Rightarrow T_c = 14.5$ K]

11. The penetration depth (λ) of Hg at 3.5 K is about 750 Å. Estimate the value of λ at $0K$. Given critical temperature (T_c) for Hg is 4.15 K. [Ans. 527.18 Å]

[Hints : $\left[\dfrac{\lambda(T)}{\lambda(0)}\right]^2 = \left[1 - \left(\dfrac{T}{T_c}\right)^4\right]^{-1}$ or $\left[\dfrac{750}{\lambda(0)}\right]^2 = \left[1 - \left(\dfrac{3.5}{4.15}\right)^4\right]^{-1} = 2.024$

or $\dfrac{750}{\lambda(0)} = 1.422$ or $\lambda(0) = 527.18$ $Å$]

12. The critical temperature of lead is $7.2K$. Determine the penetration depth of lead at 5.1 K if the penetration depth at $0K$ is 380 Å. [Ans. 439.29 Å]

[Hints : $\lambda(T) = \lambda(0)\left[1 - \left(\dfrac{T}{T_c}\right)^4\right]^{-1/2} = 380\left[1 - \left(\dfrac{5.1}{7.2}\right)^4\right]^{-1/2} = 439.29$ $Å$]

□□□

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